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A Significant Computation of Wiener Number and Hyper-Wiener Number of Graphs

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Abstract: The Wiener index of a graph G is denoted by $W(G)$ and defined as the sum of distances between all pairs of vertices in simple connected graph. Wiener index is used for modelling the shape of organic molecules and for calculating several of their physicochemical properties. In this paper we have considered the popular topological indices Wiener vector, Hyper-Wiener Vector, Wiener Matrix Sequence, Hyper Wiener Matrix sequence, Wiener number and Hyper Wiener number of graphs two connected graphs are computed and presented in a well defined form.

Keywords: Wiener matrix sequence, hyper-Wiener vector, Weighted Wiener polynomial, Wiener polynomial sequence.

I. INTRODUCTION

Let $G = (V(G), E(G))$ be a simple connected graph of order n and size m . The degree of any vertex is the number of first neighbor of v is denoted by $\deg(v)$. The distance of between any two vertices u and v of graph is defined as the length of the shortest path connecting u, v is $d(u, v)$. Topological indices are particularly suitable, if properties like shape or degree of branching are expected to have an influence on the property predicted. Calculation is often based on the distance matrix of molecular graph. A disadvantage of topological indices is that they are unrelated to observable physical properties. Quantitative structure –Activity and structure property relationships (QSAR/QSPR) use chemo-metric methods to study how a given biological activity or a physicochemical property varies as a function of topological descriptors describing the chemical structure of molecules. With these studies it is possible to replace costly and time taking biological tests or experiments of a given physiochemical property with models involving topological descriptors. In this paper we have considered the two connected graphs and their popular topological indices using the Wiener vector, Hyper-wiener Vector, Wiener Matrix Sequence, Hyper Wiener Matrix Sequence, Wiener polynomial Sequence and Hyper-wiener polynomial, Wiener number and Hyper Wiener number are calculated.

II. WIENER VECTOR AND HYPER WIENER VECTOR

For a connected graph G with n vertices, denoted by $1, 2, \dots, n$, let $W_k = \sum_{i < j, d_{ij} = k} dij$, $k=1, 2, \dots$. The vector (W_1, W_2, \dots) is called the Wiener Vector of G , denoted by $WV(G)$. Clearly, the sum of all components of the Wiener vector of G is just equal to the Wiener number of G . For a connected graph G with n vertices, denoted by $1, 2, \dots, n$, let $W_{ij,k} = \max\{d_{ij} - k + 1, 0\}$ where d_{ij} is the distance between vertices i and j . Then ${}^k W = \sum_{i < j} W_{ij,k}$, $k = 1, 2, \dots$ are called the higher Wiener numbers of G . The vector $({}^1 W, {}^2 W, \dots)$ is called the hyper-Wiener vector of G , denoted by $HWV(G)$.

Let D be the distance matrix of a connected graph of G .

Let $W^{(1)} = D$ for $k=1, 2, \dots$ $W^{(k+1)}$ is obtained from $W^{(k)}$ by leaving zeroes in place and replacing each nonzero entry x of $W^{(k)}$ by $x-1$. Let D be the distance matrix of a connected graph G , and let W^1, W^2, \dots be the Wiener matrix sequence of G . The Hyper-Wiener matrix $W^{(H)}$ of G is defined as

$$W^{(H)} = \sum_{k=1, 2, \dots} W^{(K)}$$

From the definitions, we can see that (i, j) entry of $W^{(k)}$ is just equal to $d_{ij} - k + 1$, so the sum of entries of upper triangle of $W^{(k)}$ is just equal to ${}^k W$. Moreover, the sum of entries of upper triangle of the hyper-Wiener matrix $W^{(H)}$ is just equal to the hyper-Wiener number R . However, the hyper-Wiener matrix is applicable for any connected structure.

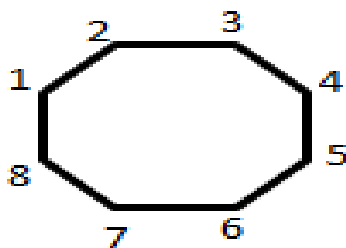


Fig 1: Graph G_1

For graph G_1 in Figure 1, its Wiener matrix sequence, Wiener vector, and hyper-Wiener vector are determined and given below.

$$W^{(1)} = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 \end{pmatrix}$$

$$W^{(2)} = \begin{pmatrix} 0 & 0 & 1 & 2 & 3 & 2 & 1 & 0 \\ 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 0 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 \\ 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 \end{pmatrix}$$

$$W^{(3)} = \begin{pmatrix} 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 \\ 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 \end{pmatrix}$$

$$W^{(4)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$W^{(H)}(G) = \begin{pmatrix} 0 & 1 & 3 & 6 & 10 & 6 & 3 & 1 \\ 1 & 0 & 1 & 3 & 6 & 10 & 6 & 3 \\ 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 \\ 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 \\ 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 \\ 6 & 10 & 6 & 3 & 1 & 0 & 1 & 3 \\ 3 & 6 & 10 & 6 & 3 & 1 & 0 & 1 \\ 1 & 3 & 6 & 10 & 6 & 3 & 1 & 0 \end{pmatrix}$$

WV(G)=(8,16,24,16), HWV(G)=(64,36,16,4), W=64, R=120.

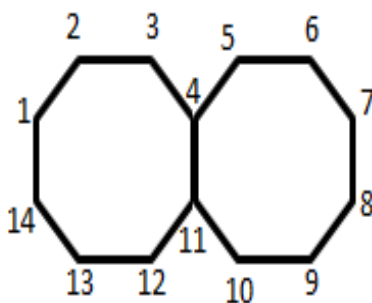


Fig 2: Graph G₂

$$W^{(1)} = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 4 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 3 & 4 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 3 & 4 & 5 \\ 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 & 4 & 5 & 6 \\ 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 5 & 4 & 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 \\ 5 & 4 & 3 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 4 & 3 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 4 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 4 & 5 & 6 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 \end{pmatrix}$$

$$W^{(2)} = \begin{pmatrix} 0 & 0 & 1 & 2 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 0 \\ 0 & 0 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 3 & 2 & 1 \\ 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 3 & 4 & 5 \\ 5 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 5 & 6 \\ 6 & 5 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 5 \\ 5 & 4 & 3 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 1 \\ 1 & 2 & 3 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 0 & 0 \\ 0 & 1 & 2 & 3 & 4 & 5 & 6 & 5 & 4 & 3 & 2 & 1 & 0 & 0 \end{pmatrix}$$

$$W^{(3)} = \begin{pmatrix} 0 & 0 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 1 & 2 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 1 & 2 \\ 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 5 \\ 5 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 2 \\ 2 & 1 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 2 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 0 & 0 \end{pmatrix}$$

$$W^{(4)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 2 \\ 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 & 4 \\ 4 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 \\ 2 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 2 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 2 & 3 & 2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 2 & 3 & 4 & 3 & 2 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

$$W^{(H)}(G) = \begin{pmatrix} 0 & 1 & 3 & 6 & 10 & 15 & 21 & 28 & 21 & 15 & 10 & 6 & 3 & 1 \\ 1 & 0 & 1 & 3 & 6 & 10 & 15 & 21 & 15 & 10 & 6 & 10 & 6 & 3 \\ 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 & 10 & 6 & 3 & 6 & 10 & 6 \\ 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 & 3 & 1 & 3 & 6 & 10 \\ 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 & 3 & 6 & 10 & 15 \\ 15 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 6 & 10 & 15 & 21 \\ 21 & 15 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 & 21 & 28 \\ 28 & 21 & 15 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 & 21 \\ 21 & 15 & 10 & 6 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 & 15 \\ 15 & 10 & 6 & 3 & 6 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 & 10 \\ 10 & 6 & 3 & 1 & 3 & 6 & 10 & 6 & 3 & 1 & 0 & 1 & 3 & 6 \\ 6 & 10 & 6 & 3 & 6 & 10 & 15 & 10 & 6 & 3 & 1 & 0 & 1 & 3 \\ 3 & 6 & 10 & 6 & 10 & 15 & 21 & 15 & 10 & 6 & 3 & 1 & 0 & 1 \\ 1 & 3 & 6 & 10 & 15 & 21 & 28 & 21 & 15 & 10 & 6 & 3 & 1 & 0 \end{pmatrix}$$

$WV(G)=\{15,36,66,72,50,36,14\}$, $HWV(G)=\{289,198,122,64,28,10,2\}$, $W=289$, $R=713$.

III. WIENER POLYNOMIAL SEQUENCE AND HYPER-WIENER POLYNOMIAL

Let D be the distance matrix of a graph G , let l be the largest entry of D , let $2d_k$ be the number of such entries of D that are equal to k . The Wiener polynomial $W(G, x)$ of G is then given by

$$W(G, x) = \sum_{k=1}^l d_k x^k$$

$W(G, x)$ related to the Wiener index of a graph G , called the Wiener polynomial $W(G, x) = \sum_{\{u,v \subseteq V(G)\}} x^{d(u,v)}$ where $d(u, v)$

denotes the distance between vertices u and v . The above two formulae give the same polynomial of G that

$$W = W'(G, 1), R = W'(G, 1) = \frac{1}{2} W''(G, 1).$$

A hyper Hosoya polynomial is given by $HH(G, x) = \sum_{k=1}^l [k + 1/2] d_k x^k$ and showed that $R(G) = HH'(G, 1)$. It can be found

that the Wiener vector (W_1, W_2, \dots) consists of the coefficients of the derivative $W'(G, x)$ of the Wiener polynomial, where W_k is equal to the coefficient $k d_k$ of x^{k-1} in $W'(G, x)$. The hyper-Wiener vector cannot be obtained from the hyper Hosoya polynomial

$HH(G, x)$. Let G be a connected graph with n vertices. The k^{th} Wiener polynomial of G , $1 \leq k \leq dia(G)$, is defined by

$$W_k(G, x) = \sum_{\{u,v \subseteq V(G)\}} x^{\max[d(u,v)-k+1, 0]}$$

, where $dia(G)$ is the diameter of G . The polynomial sequence $W_1(G, x), W_2(G, x), W_3(G, x), \dots$

IV. WIENER POLYNOMIAL SEQUENCE OF G

The weighted hyper-wiener number $R_w(G)$ of a graph G is defined as $R_w(G) = \sum_{k=1,2,\dots}^k W_{y_k}$ where y_k is the weight of $^k W$. In

addition we will introduce a novel weighted hyper-wiener polynomial $HW(G, x, y)$ of a graph G , so that the hyper-wiener vector and the weighted hyper-wiener number can be obtained from the polynomial. The Weighted hyper-Wiener polynomial $HW(G, x, y)$ of a

graph G defined as, $HW(G, x, y) = \sum_{k=1,2,\dots} W_k(G, x) y_k$ where $y = (y_1, y_2, \dots)$. From the above definition we have that

$$\frac{d}{dx}[HW(G, x, y)]/x=1 = R_w(G) = \sum_{k=1,2,\dots} k W_{Y_k}$$

where the coefficients of y_k in the weighted hyper Wiener number $R_w(G)$ are equal to the k^{th} Wiener number. Hence, the hyper-Wiener vector can be given by coefficients of $d/dx=[HW(G, x, y)]/x=1$.

In a particular graph, we have $d/dx=[HW(G, x, y)]/x=1, y=(1, 1, 1, \dots)=R(G)$

For a graph G_1 in Figure 1, the Wiener vector, the Wiener polynomial sequence, the weighted hyper Wiener polynomial of G_1 are given by

$$W'(G, x) = 16x^3 + 24x^2 + 16x + 8$$

$$WV(G) = (8, 16, 24, 16), W = 64$$

$$W^{(1)}(G, x) = 4x^4 + 8x^3 + 8x^2 + 8x$$

$$W^{(2)}(G, x) = 4x^3 + 8x^2 + 8x + 8$$

$$W^{(3)}(G, x) = 4x^2 + 8x + 16$$

$$W^{(4)}(G, x) = 4x + 24$$

$$HW(G, x, y) = (4x^4 + 8x^3 + 8x^2 + 8)y_1 + (4x^3 + 8x^2 + 8x + 8)y_2 + (4x^2 + 8x + 16)y_3 + (4x + 24)y_4$$

$$\frac{d}{dx}=[HW(G, x, y)]/x=1=64y_1+36y_2+16y_3+4y_4$$

$$\frac{d}{dx}=[HW(G, x, y)]/x=1, y=(1, 1, 1, \dots)=R(G)=120$$

For a graph G_2 in Figure 2, the Wiener vector, the Wiener polynomial sequence, the weighted hyper Wiener polynomial of G_2 are given by

$$W'(G, x) = 14x^7 + 36x^6 + 50x^5 + 72x^4 + 66x^3 + 36x^2 + 15x$$

$$WV(G) = (15, 36, 66, 72, 50, 36, 14), W = 289$$

$$W^{(1)}(G, x) = 2x^7 + 6x^6 + 10x^5 + 18x^4 + 22x^3 + 18x^2 + 15x$$

$$W^{(2)}(G, x) = 2x^6 + 6x^5 + 10x^4 + 18x^3 + 22x^2 + 18x + 15$$

$$W^{(3)}(G, x) = 2x^5 + 6x^4 + 10x^3 + 18x^2 + 22x + 33$$

$$W^{(4)}(G, x) = 2x^4 + 6x^3 + 10x^2 + 18x + 36$$

$$W^{(5)}(G, x) = 2x^3 + 6x^2 + 10x + 72$$

$$W^{(6)}(G, x) = 2x^2 + 6x + 83$$

$$W^{(7)}(G, x) = 2x + 89$$

$$\begin{aligned}
 HW(G, x, y) = & (2x^7 + 6x^6 + 10x^5 + 18x^4 + 22x^3 + 18x^2 + 15x)y_1 + \\
 & (2x^6 + 6x^5 + 10x^4 + 18x^3 + 22x^2 + 18x + 15)y_2 + \\
 & (2x^5 + 6x^4 + 10x^3 + 18x^2 + 22x + 33)y_3 \\
 & + (2x^4 + 6x^3 + 10x^2 + 18x + 36)y_4 \\
 & + (2x^3 + 6x^2 + 10x + 72)y_5 \\
 & (2x^2 + 6x + 83)y_6 + (2x + 89)y_7
 \end{aligned}$$

$$\frac{d}{dx} = [HW(G, x, y) / x=1 = 289y_1 + 198y_2 + 122y_3 + 64y_4 + 28y_5 + 10y_6 + 2y_7$$

$$\frac{d}{dx} = [HW(G, x, y) / x=1, y=(1, 1, 1, \dots) = R(G) = 713.$$

V. CONCLUSION

The topological indices are used to study quantitative structure relationships–property or activity (QSPR/QSAR). The topological invariants such as the Wiener vector, the Hyper-wiener Vector, the Wiener Matrix Sequence, the Hyper Wiener Matrix Sequence, the Wiener polynomial Sequence and the Hyper-wiener polynomial, the Wiener number and the Hyper Wiener number of graphs are derived in this work. These sequences will be helpful for similarity research analysis and multiply regression analysis in the study of structure-property relationship.

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