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Wiener Related Index of Gear Fan and Gear Wheel Related Graph

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Abstract: The modified Wiener index and I -modified hyper-Wiener index as extensions of Wiener index, are an important topological index in Chemistry. It is used for the structure of molecule. There is a very close relation between the physical, chemical characteristics of many compounds and the topological structure of that. The modified Wiener index and I -modified hyper-Wiener index are such topological indices and it has been widely used in Chemistry fields. In this paper, based on previous studies, we determine the modified Wiener index and I -modified hyper-Wiener index of gear fan graph, gear wheel graph and their r -corona graphs. The theoretical conclusions obtained in this paper illustrate the promising prospects of the application for the pharmacy and chemical engineering.

Keywords: Chemical Graph Theory; Organic Molecules; Modified Wiener Index; I -modified Hyper-Wiener Index; r -corona Graph

1. Introduction

Chemical compounds and drugs are often modeled as graphs where each vertex represents an atom of molecule, and covalent bounds between atoms are represented by edges between the corresponding vertices. This graph derived from a chemical compounds is often called its molecular graph, and can be different structures. An indicator defined over this molecular graph, the Wiener index, has been shown to be strongly correlated to various chemical properties of the compounds. The Wiener index of a graph is defined as the sum of distances between all pairs of vertices of the graph. It has been found extensive applications in chemistry. Several years later, mathematician began to pay attention to the Wiener index and study it from the mathematical point of view. In such background, since each structural feature of organic molecule can be expressed as a graph, chemical graph theory as a branch of combinatorial chemistry is introduced to research the structure of molecule from graph theory standpoint. Recently, several articles contributed to reporting certain distance-based indices of special molecular graph (See Yan et al., [1-2], Gao et al., [3-4], Gao and Shi [5], Gao and Wang [6], Xi and Gao [7-8], Xi et al., [9], Gao et al., [10] for more detail). The notation and terminology used but undefined in this paper can be found in [11].

The graphs considered in this paper are simple and connected. The vertex and edge sets of G are denoted by $V(G)$ and $E(G)$, respectively. The Wiener index is defined as the sum of distances between all unordered pair of vertices of a graph G , i.e.,

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v),$$

where $d(u,v)$ is the distance between u and v in G .

Several papers contributed to determine the Wiener index of special graphs. Chen [12] gained the exact expression for general pepoid graph. Xing and Cai [13] characterized the tree with third-minimum wiener index and introduce the method of obtaining the order of the Wiener indices among all the trees with given order and diameter, respectively. A tricyclic graph is a connected graph with n vertices and $n+2$ edges. Wan and Ren [14] studied the Wiener index of tricyclic graph t_n^3 which have at most a common vertex between any two circuits, and the smallest, the second-smallest Wiener indices of the tricyclic graphs t_n^3 are given.

The Modified Wiener index of graph G is defined by

$$W_l(G) = \sum_{\{u,v\} \subseteq V(G)} d(u,v)^l$$

The I -modified hyper-Wiener index is denoted as

$$WW_l(G) = \frac{1}{2} \left(\sum_{\{u,v\} \subseteq V(G)} d(u,v)^{2l} + \sum_{\{u,v\} \subseteq V(G)} d(u,v)^l \right)$$

Pan [15] deduced the formula of Wiener number and Hyper-Wiener number of two types of polyomino systems. More results on Wiener related index can refer to [16-23].

The graph $F_n = \{v\}P_n$ is called a fan graph and the graph $W_n = \{v\}C_n$ is called a wheel graph, where P_n is a path with n vertices and C_n is a cycle with n vertices. Graph $I_r(G)$ is called r -crown graph of G which splicing r hang edges for every vertex in G . The vertex set of hang edges

that splicing of vertex v is called r -hang vertices, note v^* . By adding one vertex in every two adjacent vertices of the fan path P_n of fan graph F_n , the resulting graph is a subdivision graph called gear fan graph, denote as $F_n^{\#}$. By adding one vertex in every two adjacent vertices of the wheel cycle C_n of wheel graph W_n , the resulting graph is a subdivision graph, called gear wheel graph, denoted as $W_n^{\#}$.

In the past ten years, the calculation of distance-based and degree-based indices for special structure of chemical molecular had raised many attention among researchers. Although there have been several advances in distance based indices of molecular graphs, the study of Wiener related indices for special chemical structures are still largely limited. In addition, as widespread and critical chemical structures, fan graph, wheel graph, gear fan graph, gear wheel graph and their r -corona graphs are widely used in medical science and pharmaceutical field. For these reasons, many kinds of indices for special structures of fan graph, wheel graph, gear fan graph, gear wheel graph and their r -corona graphs have been studied in recent years.

In this paper, we present the modified Wiener index and I -modified hyper-Wiener index of gear fan and gear wheel related graph.

2. Modified Wiener Index

Theorem 1.

$$W_1(I_r(F_n)) = (nr^2 + 2n + r - 1) + (4nr + \frac{n^2}{2} - \frac{3n}{2} + 2r - 1)2^l + ((2n - 1)r^2 + n^2 - 3n + 2)3^l + \frac{(n - 1)(n - 2)}{2}4^l.$$

Proof. Let $P_n = v_1v_2 \dots v_n$ and the r -hanging vertices of v_i be $v_i^1, v_i^2, \dots, v_i^r$ ($1 \leq i \leq n$). Let v be a vertex in F_n beside P_n , and the r -hanging vertices of v be v^1, v^2, \dots, v^r .

By the definition of modified Wiener index, we have

$$W_1(I_r(F_n)) = \sum_{i=1}^r d(v, v^i)^l + \sum_{i=1}^n d(v, v_i)^l + \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^l + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^l + \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^l = r + n + nr2^l + nr2^l + nr^23^l +$$

$$(n - 1) + \frac{(n - 1)(n - 2)}{2}2^l + nr + r((2n - 2)2^l + (n - 1)(n - 2)3^l) + nr(r - 1) + r^2((n - 1)3^l + \frac{(n - 1)(n - 2)}{2}4^l) = (nr^2 + 2n + r - 1) + (4nr + \frac{n^2}{2} - \frac{3n}{2} + 2r - 1)2^l + ((2n - 1)r^2 + n^2 - 3n + 2)3^l + \frac{(n - 1)(n - 2)}{2}4^l.$$

In this way, we get the decision.

Corollary 1. $W_1(F_n) =$

$$(2n - 1) + (\frac{n^2}{2} - \frac{3n}{2} - 1)2^l + (n^2 - 3n + 2)3^l + \frac{(n - 1)(n - 2)}{2}4^l.$$

Theorem 2.

$$W_1(I_r(W_n)) = (nr^2 + r + n^2 - n) + 4nr2^l + (2nr^2 + n^2r - 3nr)3^l + \frac{n(n - 3)r^2}{2}4^l.$$

Proof. Let $C_n = v_1v_2 \dots v_n$ and $v_i^1, v_i^2, \dots, v_i^r$ be the r -hanging vertices of v_i ($1 \leq i \leq n$). Let v be a vertex in W_n beside C_n , and v^1, v^2, \dots, v^r be the r -hanging vertices of v .

By the definition of modified Wiener index, we have

$$W_1(I_r(W_n)) = \sum_{i=1}^r d(v, v^i)^l + \sum_{i=1}^n d(v, v_i)^l + \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i^j, v_i^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^l + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^l + \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^l = r + n + nr2^l + nr2^l + nr^23^l + n(n - 2) + nr + r(2n2^l + n(n - 3)3^l) + nr(r - 1) + r^2(n3^l + \frac{n(n - 3)}{2}4^l) = (nr^2 + r + n^2 - n) + 4nr2^l + (2nr^2 + n^2r - 3nr)3^l + \frac{n(n - 3)r^2}{2}4^l.$$

Hence, we derive the desired conclusion.

Corollary 2. $W_1(W_n) = n^2 - n$.

Theorem 3.

$$W_1(I_r(F_n^{\#})) = (n + nr^2 + 5nr - 4r) + (\frac{(r^2 - r)(n - 1)}{2} - 5 + 3n + n^2 + 2nr)2^l +$$

$$(3nr^2 + 3r^2n - 3nr - 4r^2)3^l + ((\frac{n^2}{2} + \frac{3}{2}n - 3)r^2 + (\frac{3}{2}n^2 - \frac{11}{2}n + 5)4^l + ((n^2 - 3n + 2)r^2 + (n^2 - 5n + 6)r)5^l .$$

Proof. Let $P_n = v_1 v_2 \dots v_n$ and $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1} . Let $v_i^1, v_i^2, \dots, v_i^r$ be the r hanging vertices of v_i ($1 \leq i \leq n$). Let $v_{i,i+1}^1, v_{i,i+1}^2, \dots, v_{i,i+1}^r$ be the r hanging vertices of $v_{i,i+1}$ ($1 \leq i \leq n-1$). Let v be a vertex in F_n beside P_n , and the r hanging vertices of v be v^1, v^2, \dots, v^r .

By virtue of the definition of modified Wiener index, we get

$$W_l(I_r(W_n^{\text{Pn}})) = \sum_{i=1}^n d(v, v^i)^l + \sum_{i=1}^n d(v, v_i)^l + \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^l + \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_{i,i+1}^j)^l + \sum_{i=1}^{n-1} \sum_{j=1}^r d(v, v_{i,i+1}^j)^l + \sum_{i=1}^r \sum_{j=1}^{n-1} d(v^i, v_{j,j+1})^l + \sum_{i=1}^r \sum_{j=1}^{n-1} \sum_{k=1}^r d(v^i, v_{j,j+1}^k)^l + \sum_{i=1}^n \sum_{j=1}^{n-1} d(v_i, v_{j,j+1})^l + \sum_{i=1}^n \sum_{j=1}^{n-1} \sum_{k=1}^r d(v_i, v_{j,j+1}^k)^l + \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^{n-1} d(v_i^j, v_{k,k+1})^l + \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^{n-1} \sum_{t=1}^r d(v_i^j, v_{k,k+1}^t)^l + \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} d(v_{i,i+1}, v_{j,j+1})^l$$

$$+ \sum_{i=1}^{n-1} \sum_{j=1}^r d(v_{i,i+1}, v_{i,i+1}^j)^l + \sum_{i=1}^{n-1} \sum_{j \in \{1,2,L,n-1\}-i} \sum_{k=1}^r d(v_{i,i+1}, v_{j,j+1}^k)^l + \sum_{i=1}^{n-1} \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_{i,i+1}^j, v_{i,i+1}^k)^l + \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=1}^r \sum_{t=1}^r d(v_{i,i+1}^k, v_{j,j+1}^t)^l = r^2n + nr2^l + nr2^l + nr^23^l + n(n-1)2^l + nr + n(n-1)r3^l + nr(r-1) + \frac{n(n-1)}{2}r^24^l + (n-1)2^l + r(n-1)3^l + r(n-1)3^l + r^2(n-1)4^l + (2n-2)2^l + (n^2-3n+2)4^l + (2n-2+(n^2-3n+2)3^l)r + (2n-2+(n^2-3n+2)3^l)r + r^2((2n-2)3^l + (n^2-3n+2)5^l) + (n-2)2^l + \frac{(n-2)(n-3)}{2}4^l + r(r-1) + r((2n-4)3^l + (n^2-5n+6)5^l) + \frac{r(r-1)(n-1)}{2}2^l + ((n-2)4^l + \frac{(n-2)(n-3)}{2}6^l)r^2 = (n + nr^2 + 5nr - 4r) + (\frac{(r^2-r)(n-1)}{2} - 5 + 3n + n^2 + 2nr)2^l + (3nr^2 + 3r^2n - 3nr - 4r^2)3^l + ((\frac{n^2}{2} + \frac{3}{2}n - 3)r^2 + (\frac{3}{2}n^2 - \frac{11}{2}n + 5)4^l + ((n^2 - 3n + 2)r^2 + (n^2 - 5n + 6)r)5^l .$$

Thus, the result is hold.

Corollary 3. $W_l(I_r(W_n^{\text{Pn}})) = n + (-5 + 3n + n^2)2^l + (\frac{3}{2}n^2 - \frac{11}{2}n + 5)4^l .$

Theorem 4. $W_l(I_r(W_n^{\text{Pn}})) = (3n + r + 2nr) + (3nr + \frac{3}{2}n + \frac{n^2}{2} + nr^2)2^l + (3nr + 4nr^2 + n^2 + nr^2 - 2n)3^l$

$$\left(\left(\frac{n^2}{2} + \frac{3n}{2}\right)r^2 + (2n^2 - 4n)r + \frac{n^2}{2} - \frac{3n}{2}\right)4^l + \left((n^2 - 2n)r^2 + n(n-3)r\right)5^l + \frac{n(n-3)r^2}{2}6^l .$$

Proof. Let $C_n = v_1 v_2 \dots v_n$ and v be a vertex in W_n beside C_n . $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1} . Let v^1, v^2, \dots, v^r be the r hanging vertices of v and $v_i^1, v_i^2, \dots, v_i^r$ be the r hanging vertices of v_i ($1 \leq i \leq n$). Let $v_{n,n+1} = v_{1,n}$ and $v_{i,i+1}^1, v_{i,i+1}^2, \dots, v_{i,i+1}^r$ be the r hanging vertices of $v_{i,i+1}$ ($1 \leq i \leq n$). In view of the definition of Hyper-Wiener index, we deduce

$$\begin{aligned} W_1(I_r(W_n^{\mathcal{H}})) &= \sum_{i=1}^n d(v, v^i)^l + \sum_{i=1}^n d(v, v_i)^l + \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^l \\ &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^l + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^l \\ &+ \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^l + \sum_{i=1}^n d(v, v_{i,i+1})^l + \sum_{i=1}^n \sum_{j=1}^r d(v, v_{i,i+1}^j)^l \\ &+ \sum_{i=1}^r \sum_{j=1}^n d(v^i, v_{j,j+1})^l + \sum_{i=1}^r \sum_{j=1}^n \sum_{k=1}^r d(v^i, v_{j,j+1}^k)^l + \sum_{i=1}^n \sum_{j=1}^n d(v_i, v_{j,j+1})^l + \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^r d(v_i, v_{j,j+1}^k)^l \\ &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^n d(v_i^j, v_{k,k+1})^l + \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^n \sum_{t=1}^r d(v_i^j, v_{k,k+1}^t)^l \end{aligned}$$

$$\begin{aligned} &+ \sum_{i=1}^n \sum_{j=1}^r d(v_{i,i+1}, v_{i,i+1}^j)^l + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_{i,i+1}, v_{j,j+1}^k)^l + \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_{i,i+1}^j, v_{i,i+1}^k)^l \\ &+ \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_{i,i+1}^k, v_{j,j+1}^t)^l \\ &= r+n+ nr2^l + nr2^l + nr^2 3^l + \frac{n(n-1)}{2} 2^l + nr+ n(n-1)r3^l + \frac{nr(r-1)}{2} 2^l + \frac{n(n-1)r^2}{2} 4^l + n2^l + nr3^l + nr3^l + nr^2 4^l + 2n+(n^2-2n)3^l + (2n2^l + (n^2-2n)4^l)r + (2n2^l + (n^2-2n)4^l)r + (2n3^l + (n^2-2n)5^l)r^2 + n2^l + \frac{n(n-3)}{2} 4^l + rn+ (2n3^l + n(n-3)5^l)r + \frac{nr(r-1)}{2} 2^l + (n4^l + \frac{n(n-3)}{2} 6^l)r^2 \\ &= (3n+r+2nr) + (3nr+\frac{3}{2}n+\frac{n^2}{2}+nr^2)2^l + (3nr+4nr^2+n^2+nr^2-2n)3^l + \left(\left(\frac{n^2}{2} + \frac{3n}{2}\right)r^2 + (2n^2 - 4n)r + \frac{n^2}{2} - \frac{3n}{2}\right)4^l + \left((n^2 - 2n)r^2 + n(n-3)r\right)5^l + \frac{n(n-3)r^2}{2}6^l . \end{aligned}$$

As conclusion, we obtain the final conclusion.

Corollary 4. $W_1(W_n^{\mathcal{H}}) = 3n + \left(\frac{3}{2}n + \frac{n^2}{2}\right)2^l + (n^2 - 2n)3^l + \left(\frac{n^2}{2} - \frac{3n}{2}\right)4^l .$

3. 1 -Modified Hyper-Wiener Index

Theorem 5. $WW_1(I_r(F_n)) = (nr^2 + 2n + r - 1) + (4nr + \frac{n^2}{2} - \frac{3n}{2} + 2r - 1) \frac{2^l + 2^{2l}}{2}$

$$+((2n-1)r^2 + n^2 - 3n + 2) \frac{3^l + 3^{2l}}{2} + \frac{(n-1)(n-2) 4^l + 4^{2l}}{2}$$

Proof. By the definition of I -modified hyper-Wiener index, we have

$$\begin{aligned} WW_1(I_r(F_n)) &= \frac{1}{2} \left\{ \sum_{i=1}^r d(v, v^i)^l + \sum_{i=1}^n d(v, v_i)^l + \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^l \right. \\ &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^l + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^l \\ &+ \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^l \left. \right\} + \sum_{i=1}^r d(v, v^i)^{2l} + \sum_{i=1}^n d(v, v_i)^{2l} \\ &+ \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^{2l} + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^{2l} + \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^{2l} + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^{2l} \\ &+ \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^{2l} + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^{2l} + \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^{2l} \\ &+ \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^{2l} \left. \right\} \\ &= (nr^2 + 2n + r - 1) + (4nr + \frac{n^2}{2} - \frac{3n}{2} + 2r - 1) \frac{2^l + 2^{2l}}{2} \\ &+ ((2n-1)r^2 + n^2 - 3n + 2) \frac{3^l + 3^{2l}}{2} \\ &+ \frac{(n-1)(n-2) 4^l + 4^{2l}}{2} \end{aligned}$$

In this way, we get the decision.

Corollary 5. $WW_1(F_n) =$
 $(2n-1) + (\frac{n^2}{2} - \frac{3n}{2} - 1) \frac{2^l + 2^{2l}}{2}$
 $+ (n^2 - 3n + 2) \frac{3^l + 3^{2l}}{2}$
 $+ \frac{(n-1)(n-2) 4^l + 4^{2l}}{2}$

Theorem 6. $WW_1(I_r(W_n)) =$
 $(nr^2 + r + n^2 - n) + 4nr \frac{2^l + 2^{2l}}{2}$
 $+ (2nr^2 + n^2 r - 3nr) \frac{3^l + 3^{2l}}{2}$
 $+ \frac{n(n-3)r^2 4^l + 4^{2l}}{2}$

Proof. By the definition of I -modified hyper-Wiener index, we have

$$\begin{aligned} WW_1(I_r(W_n)) &= \frac{1}{2} \left\{ \sum_{i=1}^r d(v, v^i)^l + \sum_{i=1}^n d(v, v_i)^l + \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^l \right. \\ &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^l + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^l \\ &+ \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^l \left. \right\} + \sum_{i=1}^r d(v, v^i)^{2l} + \sum_{i=1}^n d(v, v_i)^{2l} \\ &+ \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^{2l} + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^{2l} + \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^{2l} + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^{2l} \\ &+ \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^{2l} + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^{2l} + \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^{2l} \\ &+ \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^{2l} \left. \right\} \\ &= (nr^2 + r + n^2 - n) + 4nr \frac{2^l + 2^{2l}}{2} \\ &+ (2nr^2 + n^2 r - 3nr) \frac{3^l + 3^{2l}}{2} \\ &+ \frac{n(n-3)r^2 4^l + 4^{2l}}{2} \end{aligned}$$

$$\begin{aligned}
 &+ \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^{2l} + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^{2l} + \\
 &\sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^{2l} \\
 &+ \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^{2l} \} \} \\
 = & \\
 &(nr^2 + r + n^2 - n) + 4nr \frac{2^l + 2^{2l}}{2} \\
 &+ (2nr^2 + n^2r - 3nr) \frac{3^l + 3^{2l}}{2} + \frac{n(n-3)r^2}{2} \frac{4^l + 4^{2l}}{2} \\
 &\dots
 \end{aligned}$$

Hence, we derivethe desire conclusion.

Corollary6. $WW_1(W_n) = n^2 - n$.

Theorem7. $WW_1(I_r(\mathbb{P}_n^{\%})) = (n + nr^2 + 5nr - 4r) +$
 $(\frac{(r^2 - r)(n - 1)}{2} - 5 + 3n + n^2 + 2nr) \frac{2^l + 2^{2l}}{2} +$
 $(3nr^2 + 3r^2n - 3nr - 4r^2) \frac{3^l + 3^{2l}}{2} +$
 $((\frac{n^2}{2} + \frac{3}{2}n - 3)r^2 + (\frac{3}{2}n^2 - \frac{11}{2}n + 5)) \frac{4^l + 4^{2l}}{2} +$
 $((n^2 - 3n + 2)r^2 + (n^2 - 5n + 6)r) \frac{5^l + 5^{2l}}{2}$.

Proof. By virtue of the definition of I -modified hyper-Wiener index, we get

$$\begin{aligned}
 WW_1(I_r(\mathbb{P}_n^{\%})) &= \frac{1}{2} \{ \sum_{i=1}^n d(v, v^i)^l + \sum_{i=1}^n d(v, v_i)^l + \\
 &\sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^l \\
 &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^l + \\
 &\sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^l + \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^l \\
 &+ \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^l + \\
 &\sum_{i=1}^{n-1} d(v, v_{i,i+1})^l + \sum_{i=1}^{n-1} \sum_{j=1}^r d(v, v_{i,i+1}^j)^l
 \end{aligned}$$

$$\begin{aligned}
 &+ \sum_{i=1}^r \sum_{j=1}^{n-1} d(v^i, v_{j,j+1})^l + \sum_{i=1}^r \sum_{j=1}^{n-1} \sum_{k=1}^r d(v^i, v_{j,j+1}^k)^l + \\
 &\sum_{i=1}^n \sum_{j=1}^{n-1} d(v_i, v_{j,j+1})^l + \sum_{i=1}^n \sum_{j=1}^{n-1} \sum_{k=1}^r d(v_i, v_{j,j+1}^k)^l \\
 &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^{n-1} d(v_i^j, v_{k,k+1})^l + \\
 &\sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^{n-1} \sum_{t=1}^r d(v_i^j, v_{k,k+1}^t)^l + \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} d(v_{i,i+1}, v_{j,j+1})^l \\
 &+ \sum_{i=1}^{n-1} \sum_{j=1}^r d(v_{i,i+1}, v_{i,i+1}^j)^l + \\
 &\sum_{i=1}^{n-1} \sum_{j \in \{1, 2, \dots, n-1\} - i} \sum_{k=1}^r d(v_{i,i+1}, v_{j,j+1}^k)^l + \\
 &\sum_{i=1}^{n-1} \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_{i,i+1}^j, v_{i,i+1}^k)^l \\
 &+ \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=1}^r \sum_{t=1}^r d(v_{i,i+1}^k, v_{j,j+1}^t)^l \} + \{ \sum_{i=1}^r d(v, v^i)^{2l} + \\
 &\sum_{i=1}^n d(v, v_i)^{2l} + \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^{2l} \\
 &+ \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^{2l} + \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^{2l} + \\
 &\sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^{2l} + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^{2l} \\
 &+ \sum_{i=1}^n \sum_{j \in \{1, 2, \dots, n\} - i} \sum_{k=1}^r d(v_i, v_j^k)^{2l} + \\
 &\sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^{2l} + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^{2l} \\
 &+ \sum_{i=1}^{n-1} d(v, v_{i,i+1})^{2l} + \sum_{i=1}^{n-1} \sum_{j=1}^r d(v, v_{i,i+1}^j)^{2l} + \\
 &\sum_{i=1}^r \sum_{j=1}^{n-1} d(v^i, v_{j,j+1})^{2l} + \sum_{i=1}^r \sum_{j=1}^{n-1} \sum_{k=1}^r d(v^i, v_{j,j+1}^k)^{2l} \\
 &+ \sum_{i=1}^n \sum_{j=1}^{n-1} d(v_i, v_{j,j+1})^{2l} + \sum_{i=1}^n \sum_{j=1}^{n-1} \sum_{k=1}^r d(v_i, v_{j,j+1}^k)^{2l} + \\
 &\sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^{n-1} d(v_i^j, v_{k,k+1})^{2l}
 \end{aligned}$$

$$\begin{aligned}
 &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^{n-1} \sum_{t=1}^r d(v_i^j, v_{k,k+1}^r)^{2l} + \\
 &\sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} d(v_{i,i+1}, v_{j,j+1})^{2l} + \sum_{i=1}^{n-1} \sum_{j=1}^r d(v_{i,i+1}, v_{i,i+1}^j)^{2l} \\
 &+ \sum_{i=1}^{n-1} \sum_{j \in \{1,2,\dots,n\}-i} \sum_{k=1}^r d(v_{i,i+1}, v_{j,j+1}^k)^{2l} + \\
 &\sum_{i=1}^{n-1} \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_{i,i+1}^j, v_{i,i+1}^k)^{2l} + \\
 &\sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=1}^r \sum_{t=1}^r d(v_{i,i+1}^k, v_{j,j+1}^t)^{2l} \} \\
 &= (n+nr^2+5nr-4r) + \\
 &(\frac{(r^2-r)(n-1)}{2} - 5 + 3n + n^2 + 2nr) \frac{2^l + 2^{2l}}{2} + \\
 &(3nr^2 + 3r^2n - 3nr - 4r^2) \frac{3^l + 3^{2l}}{2} + \\
 &((\frac{n^2}{2} + \frac{3}{2}n - 3)r^2 + (\frac{3}{2}n^2 - \frac{11}{2}n + 5)) \frac{4^l + 4^{2l}}{2} + \\
 &((n^2 - 3n + 2)r^2 + (n^2 - 5n + 6)r) \frac{5^l + 5^{2l}}{2}.
 \end{aligned}$$

Thus, the result is hold.

Corollary 7. $WW_1(\mathbb{W}_n^0) = n + (-5 + 3n + n^2) \frac{2^l + 2^{2l}}{2} + (\frac{3}{2}n^2 - \frac{11}{2}n + 5) \frac{4^l + 4^{2l}}{2}$.

Theorem 8. $WW_1(I_r(\mathbb{W}_n^0)) = (3n + r + 2nr) + (3nr + \frac{3}{2}n + \frac{n^2}{2} + nr^2) \frac{2^l + 2^{2l}}{2} + (3nr + 4nr^2 + n^2 + nr^2 - 2n) \frac{3^l + 3^{2l}}{2} + ((\frac{n^2}{2} + \frac{3n}{2})r^2 + (2n^2 - 4n)r + \frac{n^2}{2} - \frac{3n}{2}) \frac{4^l + 4^{2l}}{2} + ((n^2 - 2n)r^2 + n(n-3)r) \frac{5^l + 5^{2l}}{2} + \frac{n(n-3)r^2}{2} \frac{6^l + 6^{2l}}{3}$.

Proof. In view of the definition of I -modified hyper-Wiener index, we deduce

$$\begin{aligned}
 WW_1(I_r(\mathbb{W}_n^0)) &= \frac{1}{2} \{ \sum_{i=1}^n d(v, v^i)^l + \sum_{i=1}^n d(v, v_i)^l + \\
 &\sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^l + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^l \\
 &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^l + \\
 &\sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^l + \sum_{i=1}^n \sum_{j \in \{1,2,\dots,n\}-i} \sum_{k=1}^r d(v_i, v_j^k)^l \\
 &+ \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^l + \sum_{i=1}^n \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^l + \\
 &\sum_{i=1}^n d(v, v_{i,i+1})^l + \sum_{i=1}^n \sum_{j=1}^r d(v, v_{i,i+1}^j)^l \\
 &+ \sum_{i=1}^r \sum_{j=1}^n d(v^i, v_{j,j+1})^l + \sum_{i=1}^r \sum_{j=1}^n \sum_{k=1}^r d(v^i, v_{j,j+1}^k)^l + \\
 &\sum_{i=1}^n \sum_{j=1}^n d(v_i, v_{j,j+1})^l + \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^r d(v_i, v_{j,j+1}^k)^l \\
 &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^n d(v_i^j, v_{k,k+1})^l + \\
 &\sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r \sum_{t=1}^r d(v_i^j, v_{k,k+1}^t)^l + \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_{i,i+1}, v_{j,j+1})^l \\
 &+ \sum_{i=1}^n \sum_{j=1}^r d(v_{i,i+1}, v_{i,i+1}^j)^l + \\
 &\sum_{i=1}^n \sum_{j \in \{1,2,\dots,n\}-i} \sum_{k=1}^r d(v_{i,i+1}, v_{j,j+1}^k)^l + \\
 &\sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_{i,i+1}^j, v_{i,i+1}^k)^l \\
 &+ \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_{i,i+1}^k, v_{j,j+1}^t)^l \} + \{ \sum_{i=1}^r d(v, v^i)^{2l} + \\
 &\sum_{i=1}^n d(v, v_i)^{2l} + \sum_{i=1}^n \sum_{j=1}^r d(v, v_i^j)^{2l} \\
 &+ \sum_{i=1}^n \sum_{j=1}^r d(v_i, v^j)^{2l} + \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^r d(v_i^j, v^k)^{2l} + \\
 &\sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_i, v_j)^{2l} + \sum_{i=1}^n \sum_{j=1}^r d(v_i, v_i^j)^{2l}
 \end{aligned}$$

$$\begin{aligned}
& + \sum_{i=1}^n \sum_{j \in \{1,2,L,n\}-i} \sum_{k=1}^r d(v_i, v_j^k)^{2l} + \\
& \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_i^j, v_i^k)^{2l} + \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_i^k, v_j^t)^{2l} \\
& + \sum_{i=1}^n d(v, v_{i,i+1})^{2l} + \sum_{i=1}^n \sum_{j=1}^r d(v, v_{i,i+1}^j)^{2l} + \\
& \sum_{i=1}^r \sum_{j=1}^n d(v^i, v_{j,j+1})^{2l} + \sum_{i=1}^r \sum_{j=1}^n \sum_{k=1}^r d(v^i, v_{j,j+1}^k)^{2l} \\
& + \sum_{i=1}^n \sum_{j=1}^n d(v_i, v_{j,j+1})^{2l} + \sum_{i=1}^n \sum_{j=1}^n \sum_{k=1}^r d(v_i, v_{j,j+1}^k)^{2l} + \\
& \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^n d(v_i^j, v_{k,k+1})^{2l} \\
& + \sum_{i=1}^n \sum_{j=1}^r \sum_{k=1}^n \sum_{t=1}^r d(v_i^j, v_{k,k+1}^t)^{2l} + \\
& \sum_{i=1}^{n-1} \sum_{j=i+1}^n d(v_{i,i+1}, v_{j,j+1})^{2l} + \sum_{i=1}^n \sum_{j=1}^r d(v_{i,i+1}, v_{i,i+1}^j)^{2l} \\
& + \sum_{i=1}^n \sum_{j \in \{1,2,L,n\}-i} \sum_{k=1}^r d(v_{i,i+1}, v_{j,j+1}^k)^{2l} + \\
& \sum_{i=1}^n \sum_{j=1}^{r-1} \sum_{k=j+1}^r d(v_{i,i+1}^j, v_{i,i+1}^k)^{2l} + \\
& \sum_{i=1}^{n-1} \sum_{j=i+1}^n \sum_{k=1}^r \sum_{t=1}^r d(v_{i,i+1}^k, v_{j,j+1}^t)^{2l} \} \}
\end{aligned}$$

$$\begin{aligned}
& = (3n + r + 2nr) + (3nr + \frac{3}{2}n + \frac{n^2}{2} + nr^2) \frac{2^l + 2^{2l}}{2} \\
& + (3nr + 4nr^2 + n^2 + nr^2 - 2n) \frac{3^l + 3^{2l}}{2} + \\
& ((\frac{n^2}{2} + \frac{3n}{2})r^2 + (2n^2 - 4n)r + \frac{n^2}{2} - \frac{3n}{2}) \frac{4^l + 4^{2l}}{2} + \\
& ((n^2 - 2n)r^2 + n(n-3)r) \frac{5^l + 5^{2l}}{2} + \\
& \frac{n(n-3)r^2}{2} \frac{6^l + 6^{2l}}{3}.
\end{aligned}$$

As conclusion, we obtain the final conclusion.

Corollary 8. $WW_1(W_n^{\circ}) = 3n + (\frac{3}{2}n + \frac{n^2}{2}) \frac{2^l + 2^{2l}}{2} +$

$$(n^2 - 2n) \frac{3^l + 3^{2l}}{2} + (\frac{n^2}{2} - \frac{3n}{2}) \frac{4^l + 4^{2l}}{2}.$$

4. Conclusion

Combinatorial chemistry is a new powerful technology in molecular recognition and drug design. It is a wet-laboratory methodology purposed to massively parallel screening of chemical compounds for the founding of compounds that have certain biological activities. The power of trick draws from the interaction between computational modeling and experimental design.

Fan graph, wheel graph, gear fan graph, gear wheel graph and their r -corona graphs are common structural features of organic molecules. The contributions of our paper are determining the l -modified Wiener index and l -modified hyper-Wiener index of these special structural features of organic molecules.

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