Total Szeged Index, Vertex-Edge Wiener Index and Edge Hyper-Wiener Index of Certain Special Molecular Graphs

Yun Gao1, * , Zhiyang Jia2, Wei Gao3

1Department of Editorial, Yunnan Normal University, Kunming, China
2Tourism and culture college, Yunnan University, Lijiang, China
3School of Information Science and Technology, Yunnan Normal University, Kunming, China

Abstract

In past years, topological indices are introduced to measure the characters of chemical molecules. Thus, the study of these topological indices has raised large attention in the field of chemical science, biology science and pharmaceutical science. In this paper, by virtue of molecular structure analysis, we determine the total Szeged index, vertex-edge Wiener index and edge hyper-Wiener index of several crucial molecular graphs, such as fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs. The results achieved in our paper illustrate the promising application prospects for chemical engineering.

Keywords

Chemical Graph Theory, Total Szeged Index, Vertex-Edge Wiener Index, Edge Hyper-Wiener Index, Fan Molecular Graph, Wheel Molecular Graph, Gear Fan Molecular Graph, Gear Wheel Molecular Graph, r-Corona Molecular Graph

1. Introduction

Wiener index, PI index and Zagreb indices are introduced to reflect certain structural features of organic molecules. Several papers contributed to determine the distance-based index of special molecular graphs (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).

Let $e=uv$ be an edge of the molecular graph $G$. The number of edges and vertices of $G$ whose distance to the vertex $u$ is smaller than the distance to the vertex $v$ is denoted by $t_u(e)$.

Analogously, $t_v(e)$ is the number of edges and vertices of $G$ whose distance to the vertex $v$ is smaller than the distance to the vertex $u$. The total Szeged index of $G$ is defined as

$$S_{Tz}(G) = \sum_{e \in G} t_u(e)t_v(e).$$

Manuel et al., [11] determined the total Szeged Index of C4-Nanotubes, C4-Nanotori and Dendrimer Nanostars. It is well know that

$$S_{Tz}(G) = S_{ez}(G) + S_{zv}(G) + 2S_{ev}(G),$$

where $S_{ez}(G)$ is edge-Szeged index, $S_{zv}(G)$ is vertex-Szeged index, and $S_{ev}(G)$ is edge-vertex Szeged index.

Let $u$ be a vertex in molecular graph $G$. For the edges $e=ab$ and $f=xy$, let

$$d'(u,e) = D'(e,u) = \min\{d(u,a),d(u,b)\}$$

* Corresponding author
E-mail address: gaoyun@ynnu.edu.cn (Yun Gao)
and
\[ D(e, f) = \min \{D(e, x), D(e, y)\}. \]

The vertex-edge Wiener index is introduced by Cevik and Maden [12] as follows:
\[ W_{\alpha}(G) = \frac{1}{2} \sum_{i \in E(G)} d(i, f). \]

Similar as Wiener index and hyper-Wiener index, we define the edge hyper-Wiener index of molecular graph \( G \) as follows
\[ WW_{\alpha}(G) = \frac{1}{2} \sum_{i \in E(G)} \{d(e, f) + d^2(e, f)\}. \]

Let \( P_n \) and \( C_n \) be path and cycle with \( n \) vertices. The molecular graph \( F_n = \{v\} \bigvee P_n \) is called a fan molecular graph and the molecular graph \( W_n = \{v\} \bigvee C_n \) is denoted as a wheel molecular graph. Molecular graph \( I_1(G) \) is called \( r \)-crown molecular graph of \( G \) which splicing \( r \) hanging edges for every vertex in \( G \). By adding one vertex in every two adjacent vertices of the fan path \( P_n \) of fan molecular graph \( F_n \), the resulting molecular graph is a subdivision molecular graph called gear fan molecular graph, denote as \( \tilde{F}_n \). By adding one vertex in every two adjacent vertices of the wheel cycle \( C_n \) of wheel molecular graph \( W_n \), the resulting molecular graph is a subdivision molecular graph, called gear wheel molecular graph, denoted as \( \tilde{W}_n \).

As we know, fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph and \( r \)-corona molecular graph are common molecular structure in chemical. Hence, it inspires us to study the topological indices of these important chemical molecular structures. In this paper, we present the total Szeged index, vertex-edge Wiener index and edge hyper-Wiener index of \( I_1(F_n) \), \( I_1(W_n) \), \( I_1(\tilde{F}_n) \) and \( I_1(\tilde{W}_n) \). The rest parts of the article are organized as follows: first, we compute the total Szeged index of above molecular graphs; then, the vertex-edge Wiener index of such chemical structures are presented; at last, we derive the edge hyper-Wiener index of these special molecular graphs.

### 2. Total Szeged Index

**Theorem 1.** \( \text{Sz}_e(I_1(F_n)) = r^n(8n^2 + 16n - 18) + (18n^2 + 14n - 62) + (9n^2 - 32). \)

**Proof.** Let \( P_n = v_1v_2 \ldots v_n \) and the \( r \) hanging vertices of \( v_i \) be \( v_i^1, v_i^2, \ldots, v_i^r \) \((1 \leq i \leq n)\). Let \( v \) be a vertex in \( F_n \) beside \( P_n \), and the \( r \) hanging vertices of \( v \) be \( v_i^1, v_i^2, \ldots, v_i^r \). Using the definition of total Szeged index, we have

**Corollary 1.** \( \text{Sz}_e(F_n) = 9n^2 - 32 \).

**Theorem 2.** \( \text{Sz}_e(I_1(W_n)) = r^n(6n^2 + 24n - 4) + r(12n^2 + 43n - 28) + (5n^2 + 21n - 18) \).

**Proof.** Let \( C_n = v_1v_2 \ldots v_n \) and \( v_i^1, v_i^2, \ldots, v_i^r \) 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 \( v_i^1, v_i^2, \ldots, v_i^r \) be the \( r \) hanging vertices of \( v \). We denote \( v_{v_i,v_i^1} = v_i^1 v_i \). In view of the definition of total Szeged index, we infer

\[ \text{Sz}_e(I_1(W_n)) = \sum_{i=1}^{n} (t_i(v_{i,v_i}^1) + v_i^1) + \sum_{i=1}^{n} (t_i(v_{i,v_i}^2) + v_i^2) + \sum_{i=1}^{n} (t_i(v_{i,v_i}^r) + v_i^r) \]

and

\[ \text{Sz}_e(\tilde{F}_n) = \sum_{i=1}^{n} (t_i(v_{i,v_i}^1) + v_i^1) + \sum_{i=1}^{n} (t_i(v_{i,v_i}^2) + v_i^2) + \sum_{i=1}^{n} (t_i(v_{i,v_i}^r) + v_i^r) \]

and

\[ \text{Sz}_e(\tilde{W}_n) = \sum_{i=1}^{n} (t_i(v_{i,v_i}^1) + v_i^1) + \sum_{i=1}^{n} (t_i(v_{i,v_i}^2) + v_i^2) + \sum_{i=1}^{n} (t_i(v_{i,v_i}^r) + v_i^r) \]

As we know, fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph and \( r \)-corona molecular graph are common molecular structure in chemical. Hence, it inspires us to study the topological indices of these important chemical molecular structures. In this paper, we present the total Szeged index, vertex-edge Wiener index and edge hyper-Wiener index of \( I_1(F_n) \), \( I_1(W_n) \), \( I_1(\tilde{F}_n) \) and \( I_1(\tilde{W}_n) \). The rest parts of the article are organized as follows: first, we compute the total Szeged index of above molecular graphs; then, the vertex-edge Wiener index of such chemical structures are presented; at last, we derive the edge hyper-Wiener index of these special molecular graphs.
Corollary 2. \( S_T(F_n) = 5n^2 + 21n - 18 \).

Theorem 3. \( S_T(T_n(F_n^r)) = r^2(88n^2 - 156n + 96) + r(170n^2 - 390n + 240) + (75n^2 - 204n + 134) \).

Proof. Let \( P_n = v_1, v_2, \ldots, v_n \) and \( v_{r+1}, \ldots, v_{r+n} \) be the hanging vertices of \( v \) (1 ≤ i ≤ n). Let \( v_1, v_2, \ldots, v_r \) be the r hanging vertices of \( v_i \). In view of the definition of total Szeged index, we deduce

\[
S_T(T_n(F_n^r)) = \sum_{i=1}^{r} (t_i(v,v_i)t_i(v^r)) + \sum_{j=1}^{r} (t_j(v,v_j)t_j(v^r)) + \sum_{i=1}^{r} \sum_{j=1}^{r} (t_i(v,v_i)t_j(v^r)) + \sum_{i=1}^{r} \sum_{j=1}^{r} (t_i(v,v_i)t_j(v^r))
\]

By virtue of the definition of total Szeged index, we yield

\[
S_T(T_n(F_n^r)) = \sum_{i=1}^{r} (t_i(v,v_i)t_i(v^r)) + \sum_{j=1}^{r} (t_j(v,v_j)t_j(v^r)) + \sum_{i=1}^{r} \sum_{j=1}^{r} (t_i(v,v_i)t_j(v^r)) + \sum_{i=1}^{r} \sum_{j=1}^{r} (t_i(v,v_i)t_j(v^r))
\]

Corollary 3. \( S_T(F_n) = 75n^2 - 204n + 134 \).

Theorem 4. \( S_T(T_n(F_n^r)) = r^2(88n^2 - 60n + 2) + r(170n^2 - 169n + 3) + (75n^2 - 95n - 2) \).

Proof. Let \( C_n = v_1, v_2, \ldots, v_n \) and \( v \) be a vertex in \( W_n \) beside \( C_n \) and \( v_{r+1}, \ldots, v_{r+n} \) be the hanging vertices of \( v \). In view of the definition of total Szeged index, we deduce

\[
S_T(T_n(F_n^r)) = \sum_{i=1}^{r} (t_i(v,v_i)t_i(v^r)) + \sum_{j=1}^{r} (t_j(v,v_j)t_j(v^r)) + \sum_{i=1}^{r} \sum_{j=1}^{r} (t_i(v,v_i)t_j(v^r)) + \sum_{i=1}^{r} \sum_{j=1}^{r} (t_i(v,v_i)t_j(v^r))
\]

Corollary 4. \( S_T(F_n) = 75n^2 - 204n + 134 \).
Corollary 4. \( Sz_j(W_e) = 75n^2 - 95n - 2 \).

3. Vertex-Edge Wiener Index

The notations and terminologies for particular molecular graphs presented in this section can refer to section 2.

Theorem 5. \( W_{ev}(I(F_q)) = r^2 \left( \frac{3}{2}n^2 - \frac{1}{2}n + \frac{3}{2} + r^2 - n^2 - 2n + 2 + \frac{2}{2}n^2 - 4n + 2 \right) \).

Proof. Using the definition of vertex-edge Wiener index, we have

\[
W_{ev}(I(F_q)) = \frac{1}{2} \left( \sum_{i=1}^{r} d'(v, v') + \sum_{i=1}^{r} d'(v', v) + \sum_{i=1}^{r} d'(v' ,vv') + \sum_{i=1}^{r} d'(v', v) + \sum_{i=1}^{r} d'(v', v) + \sum_{i=1}^{r} d'(v', v) + \sum_{i=1}^{r} d'(v', v) \right)
\]

\[
+ \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v, v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j)
\]

\[
= \frac{1}{2} \left( 0 + (r^2 - r) + nr^2 + 0 + nr + (n^2 - n) + r(2n^2 - n) + (n - 1) + r(2n - 2) + (2n^2 - 8n + 5) + r(3n^2 - 9n + 5) + nr + 2nr^2 + r(2n^2 - 4n + 2) + r^2(3n^2 - 5n + 2) \right)
\]

\[
= r^2 \left( \frac{3}{2}n^2 - \frac{1}{2}n + \frac{3}{2} + r^2 - n^2 - 2n + 2 + \frac{2}{2}n^2 - 4n + 2 \right) \).
\]

Corollary 5. \( W_{ev}(F_n) = \frac{3}{2}n^2 - 4n + 2 \).

Theorem 6. \( W_{ev}(I(W_q)) = r^2 \left( \frac{3}{2}n^2 - \frac{1}{2}n + \frac{3}{2} + r^2 - n^2 - 2n + 2 + \frac{2}{2}n^2 - 3n \right) \).

Proof. In view of the definition of vertex-edge Wiener index, we infer

\[
W_{ev}(I(W_q)) = \frac{1}{2} \left( \sum_{i=1}^{r} d'(v, v') + \sum_{i=1}^{r} d'(v', v) + \sum_{i=1}^{r} d'(v' ,vv') + \sum_{i=1}^{r} d'(v', v) + \sum_{i=1}^{r} d'(v', v) + \sum_{i=1}^{r} d'(v', v) + \sum_{i=1}^{r} d'(v', v) \right)
\]

\[
+ \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v, v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j) + \sum_{i=1}^{r} \sum_{j=1}^{n} d'(v', v_j)
\]

\[
= \frac{1}{2} \left( 0 + (r^2 - r) + nr^2 + 0 + nr + (n^2 - n) + r(3n^2 - 4n) + n + 2nr + (2n^2 - 6n) + r(3n^2 - 6n) + nr + 2nr^2 + r(2n^2 - 4n) + r^2(3n^2 - 5n) \right)
\]

\[
= r^2 \left( \frac{3}{2}n^2 - \frac{1}{2}n + \frac{1}{2} + r(4n^2 - \frac{9}{2}n - \frac{1}{2}) + \frac{3}{2}n^2 - 3n \right) \).
Corollary 6. \( W_n(W_n) = \frac{3}{2} n^2 - 3n \).

Theorem 7. \( W_n(I_n(\tilde{F}_n)) = r^2 (8n^2 - 14n + \frac{21}{2}) + r (\frac{31}{2} n^2 - \frac{67}{2} n + \frac{45}{2}) + (\frac{13}{2} n^2 - \frac{33}{2} n + 13) \).

Proof. By virtue of the definition of vertex-edge Wiener index, we yield

\[
W_n(I_n(\tilde{F}_n)) = \frac{1}{2} \left( \sum_{i,j,k} d'(v_i,v_j) + \sum_{i,j,k} d'(v_i,v_k) + \sum_{i,j,k} d'(v_j,v_k) + \sum_{i,j,k} d'(v_i,v_j) + \sum_{i,j,k} d'(v_j,v_k) + \sum_{i,j,k} d'(v_i,v_k) \right)
\]

\[
+ \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k)
\]

\[
+ \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k)
\]

\[
+ \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k)
\]

\[
+ \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k)
\]

\[
+ \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k) + \sum_{i,j,k} d'(v_j,v_i,v_k) + \sum_{i,j,k} d'(v_i,v_j,v_k)
\]

\[
= \frac{1}{2} \left[ 0 + r^2 - r + r + 2n + 2nr + r(2n - 2) + r^2 (3n - 3) + 0 + r + (n^2 - n) + r(2n^2 - n) + (2n^2 - 4n + 2)
\]

\[
+ r(3n^2 - 5n + 2) + (n - 1) + r(2n - 2) + (2n^2 - 3n + 1) + r(3n^2 - 6n + 1) + (3n^2 - 12n + 1) + r(4n^2 - 14n + 13)
\]

\[
+ (n - 1) + r(2n - 2) + (2n^2 - 3n + 1) + r(3n^2 - 6n + 1) + (3n^2 - 12n + 1) + r(4n^2 - 14n + 13) + r + 2nr^2
\]

\[
+ r(2n^2 - 2n) + r^2 (3n^2 - 3n) + r(3n^2 - 7n + 4) + r^2 (4n^2 - 8n + 4) + r(2n - 2) + r^2 (3n - 3) + r(3n^2 - 7n + 4)
\]

\[
+ r^2 (4n^2 - 8n + 4) + r(4n^2 - 16n + 16) + r^2 (5n^2 - 19n + 18)
\]

\[
= r^2 (8n^2 - 14n + \frac{21}{2}) + r (\frac{31}{2} n^2 - \frac{67}{2} n + \frac{45}{2}) + (\frac{13}{2} n^2 - \frac{33}{2} n + 13).
\]

Corollary 7. \( W_n(\tilde{F}_n) = \frac{13}{2} n^2 - \frac{33}{2} n + 13 \).

Theorem 8. \( W_n(I_n(\tilde{W}_n)) = r^2 (8n^2 - 4n + \frac{1}{2}) + r (\frac{31}{2} n^2 - 15n - \frac{1}{2}) + (\frac{13}{2} n^2 - 19 n) \).

Proof. In view of the definition of vertex-edge Wiener index, we deduce
\[
W_{\varepsilon}(I_{\bar{F}_n}) = \frac{1}{2} \left( \sum_{i=1}^{n} d'(v, v') + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_j, v_j') + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_k', v_k') + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_k, v_k') + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_{j,i}, v_{j,i}') \right) 
\]

\[
+ \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_{j,i}, v_{j,i}') + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_j, v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_k', v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_k, v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_{j,i}, v_{j,i}') \]

\[
+ \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_{j,i}, v_{j,i}') + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_j, v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_k', v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_k, v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_{j,i}, v_{j,i}') \]

\[
+ \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_{j,i}, v_{j,i}') + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_j, v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_k', v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_k, v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_{j,i}, v_{j,i}') \]

\[
+ \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_{j,i}, v_{j,i}') + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_j, v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} d'(v_k', v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_k, v_{j,i}) + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d'(v_{j,i}, v_{j,i}') \]

\[
+ \frac{1}{2} \left( 0 + (r^2 - r) + r + 2n^2 + 2nr + 3n^2 + 0 + r^2 - n + r(2n^2 - n) + (2n^2 - n) + r(3n^2 - 2n) + n + 2nr \\
+ (2n^2 - 3n) + r(3n^2 - 3n) + (3n^2 - 6n) + r(4n^2 - 6n) + n + 2nr + (2n^2 - 3n) + r(3n^2 - 3n) + (3n^2 - 6n) \\
+ r(4n^2 - 6n) + r + 2nr + r(2n^2 - 2n) + r(3n^2 - 3n) + r(3n^2 - 4n) + r^2(4n^2 - 4n) + 2nr + 2nr + r^2(3n^2 - 4n) \\
+ r^2(4n^2 - 4n) + r(4n^2 - 8n) + r^2(5n^2 - 9n) \right) 
\]

\[
= r^2(8n^2 - 4n + \frac{1}{2}) + r + \frac{3n^2}{2} - 15n - \frac{1}{2} + (\frac{13}{2}n^2 - \frac{19}{2}n) 
\]

Corollary 8. \( W_{\varepsilon}(\bar{F}_n) = \frac{13}{2}n^2 - \frac{19}{2}n \).

4. Edge Hyper-Wiener Index

The notations and terminologies for special molecular graphs used in this section can refer to section 2.

Theorem 9. \( WW_{\varepsilon}(I_{\bar{F}_n}) = r^2(3n^2 - \frac{5}{2}n + \frac{7}{2}) + r(9n^2 - 21n + 18) + (\frac{13}{2}n^2 - \frac{49}{2}n + 29) \).

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

\[
WW_{\varepsilon}(I_{\bar{F}_n}) = \frac{1}{2} \left( \sum_{i=1}^{n} \sum_{j=1}^{n} d(v', v') + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} d(v_j', v_j') + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{l=1}^{n} d(v_j', v_l') + \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{l=1}^{n} \sum_{m=1}^{n} d(v_j', v_m') \right) 
\]
Theorem 10. By the definition of edge hyper-Wiener index, we have

\[ WW(F) = \frac{1}{2} \left( r^2 \left( r(n-1) + \frac{nr(r-1)}{2} + \frac{r^2}{2} \left( \frac{3}{2} n^2 - \frac{5}{2} \right) + 2nr^2 + 2r(n-1) + r(2n^2 - n) + r(3n^2 - 9n + 8) \right) \right) \]

\[ + \frac{n(n-1)}{2} \left( \frac{3}{2} n^2 - \frac{15}{2} + 10 \right) + \left( 2n^2 - 4n + 2 \right) \] + \left( \frac{r(r-1)}{2} + \frac{nr(r-1)}{2} + \frac{r^2}{2} \left( \frac{9}{2} n^2 - \frac{19}{2} \right) + 5 \right) + 4nr^2

\[ + rn + 4r(n-1) + r(4n^2 - 3n) + r(9n^2 - 35n + 36) + \left( \frac{n(n-1)}{2} + \frac{9}{2} n^2 - \frac{53}{2} + 40 \right) \] + \left( 4n^2 - 10n + 6 \right) \}

Corollary 9. \( WW(F_n) = \frac{13}{2} n^2 - \frac{49}{2} + 2n + 29 \).

Theorem 10. \( WW(I(F_n)) = r^2 \left( 3n^2 - \frac{5}{2} n + \frac{1}{2} \right) + r(9n^2 - \frac{29}{2} n - \frac{1}{2}) + \left( \frac{13}{2} n^2 - \frac{31}{2} n \right) \).

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

\[ WW(F_n) = \frac{1}{2} \left( \frac{r^2}{2} \left( \frac{3}{2} n^2 - \frac{5}{2} \right) + 2nr^2 + 2r(n-1) + r(2n^2 - n) + r(3n^2 - 9n + 8) \right) \]

\[ + \frac{n(n-1)}{2} \left( \frac{3}{2} n^2 - \frac{15}{2} + 10 \right) + \left( 2n^2 - 4n + 2 \right) \] + \left( \frac{r(r-1)}{2} + \frac{nr(r-1)}{2} + \frac{r^2}{2} \left( \frac{9}{2} n^2 - \frac{19}{2} \right) + 5 \right) + 4nr^2

\[ + rn + 4r(n-1) + r(4n^2 - 3n) + r(9n^2 - 35n + 36) + \left( \frac{n(n-1)}{2} + \frac{9}{2} n^2 - \frac{53}{2} + 40 \right) \] + \left( 4n^2 - 10n + 6 \right) \}

\[ = r^2 \left( 3n^2 - \frac{5}{2} n + \frac{7}{2} \right) + r(9n^2 - 21n + 18) + \left( \frac{13}{2} n^2 - \frac{49}{2} n + 29 \right) \].
Corollary 10. \( WW'(W_n) = \frac{13}{2} n^2 - \frac{31}{2} n \).

Theorem 11. \( WW'(I(F)) = r^3 (\frac{41}{2} n^2 - 53n + \frac{83}{2}) + r(41n^2 - 144n + 98) + (\frac{37}{2} n^2 - \frac{115}{2} n + 45) \).

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

\[
WW'(I(F)) = \frac{1}{2} \left( \sum_{i,j} d(v_i, v_j) + \sum_{i,j} d(v_i, v'_j) + \sum_{i,j} d(v'_i, v'_j) + \sum_{i,j} d(v_i, v'_i) + \sum_{i,j} d(v'_i, v'_i) \right) + \sum_{i,j} d(v_i, v_j) + \sum_{i,j} d(v_i, v'_j) + \sum_{i,j} d(v'_i, v_j) + \sum_{i,j} d(v'_i, v'_j)
\]
Proof. Corollary 11. \[ W_{W,1} = \frac{37}{2} n^2 - \frac{115}{2} n + 45. \]

Theorem 12. \[ W_{W,1}(I, \vec{w}) = r^2 \left( \frac{41}{2} n^2 - \frac{47}{2} n + \frac{1}{2} \right) + r(41n^2 - 58n - \frac{1}{2} + \frac{37}{2} n^2 - \frac{63}{2} n). \]

Proof. In view of the definition of edge hyper-Wiener index, we deduce
\[\sum_{i=1}^{n} \sum_{j=1}^{n} d(v_i,v_j) + \sum_{i=1}^{n} \sum_{j=1}^{n} d(v_i',v_j') + \sum_{i=1}^{n} \sum_{j=1}^{n} d(v_i,v_j') + \sum_{i=1}^{n} \sum_{j=1}^{n} d(v_i',v_j)\]

\[= n(n-1) + \frac{n^2(n-1)}{2}\]

**Corollary 12.** \(WW(W_{1}) = \frac{37}{2} n^2 - \frac{63}{2} n\).

## 5. Future Work

Let \(e_v(v)\) be the eccentricity of a vertex \(v\) in a connected molecular graph \(G\), \(n=|V(G)|\) be a number of vertices, and \(m=|E(G)|\) be a number of edges. Cevik and Maden [12] defined following average class of molecular graph...
invariants:

- Average eccentricity: \( avec(G) = \frac{1}{n} \sum_{v \in V(G)} e_v(v) = \frac{1}{n} \sum_{v \in V(G)} \max_{u \in V(G)} d(u, v). \)

- Average edge eccentricity: \( avec_e(G) = \frac{1}{m} \sum_{e \in E(G)} \max_{f \in E(G)} D(g, f). \)

- Average vertex-edge eccentricity: \( avec_{ve}(G) = \frac{1}{n} \sum_{v \in V(G)} \max_{f \in E(G)} d'(v, f). \)

- Weighted average eccentricity: \( avec_{w}(G) = \frac{1}{n} \sum_{v \in V(G)} \deg(v) e_v(v). \)

Hence, these average indices of special structural molecules graphs can be consider as subjects for future research.

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