Logarithm Multiplicative Wiener Index and Reciprocal Complementary Wiener Index of Certain Special Molecular Graphs

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Abstract
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. In this paper, we determine the logarithm multiplicative Wiener index and reciprocal complementary Wiener index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs.

Keywords
Chemical Graph Theory, Logarithm Multiplicative Wiener Index, Reciprocal Complementary Wiener Index, r-Corona Molecular Graph

1. Introduction
Wiener index, Gutman index, Shultz index, Geometric-arithmetic index and Zagreb indices are introduced to reflect certain structural features of organic molecules. Several papers contributed to determine the distance-based index or degree-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). The notation and terminology used but undefined in this paper can be found in [11].

Gutman et al., [12] introduced the logarithm of multiplicative Wiener index of molecular graph $G$ as:

$$\Pi(G) = \ln\left(2 \prod_{\{u,v\} \in G} d(u,v)\right)$$

Let $D = D(G)$ be the diameter of molecular graph $G$. Parallel to the Wiener index, the reciprocal complementary Wiener (RCW) index is defined by [13] as

$$RCW(G) = \sum_{\{u,v\} \in G} \frac{1}{1 + D - d(u,v)}$$

Let $P_n$ and $C_n$ be path and cycle with $n$ vertices. The molecular graph $F_n = \{v\} \lor P_n$ is called a fan molecular graph and the molecular graph $W_n = \{v\} \lor C_n$ is called a wheel molecular graph. Molecular graph $I_r(G)$ is called $r$- crown molecular graph of $G$ which splicing $r$ hangs 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 $\tilde{W}_n$. 

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In this paper, we present the logarithm multiplicative Wiener index and reciprocal complementary Wiener index of $I_r(F_n)$, $I_r(F_n^r)$ and $I_r(W_n)$.

2. Logarithm Multiplicative Wiener Index

Theorem 1. \[ \Pi(I_r(F_n)) = \text{Ln} \left( \sqrt{2^{(n-1)(n-2) + (n-1)(n-3)}} \cdot \text{Ln} \left( \sqrt{2^{(n-1)(n-2) + (n-1)(n-3) + (n-1)(n-2)}} \right) \right). \]

Proof. Let $P_n=v_1v_2…v_n$ and the $r$ hanging vertices of $vi$, $v_i^1$, $v_i^2$, …, $v_i^r$ $(1 \leq i \leq n)$. Let $v$ be a vertex in $F_n$ beside $P_n$, and the $r$ hanging vertices of $v$ be $v^1$, $v^2$, …, $v^r$. By the definition of logarithm multiplicative Wiener index, we have

\[ \Pi(I_r(F_n)) = \text{Ln}(\sqrt{2^{(n-1)(n-2) + (n-1)(n-3) + (n-1)(n-2)}} \cdot \text{Ln} \left( \sqrt{2^{(n-1)(n-2) + (n-1)(n-3) + (n-1)(n-2)}} \right)). \]

Corollary 1. \[ \Pi(F_n^r) = \text{Ln} \left( \sqrt{2^{(n-1)(n-2) + (n-1)(n-3)}} \right). \]

Theorem 2. \[ \Pi(I_r(W_n)) = \text{Ln} \left( \sqrt{2^{n(n-1) + n(n-2) + n(n-3)}} \cdot \text{Ln} \left( \sqrt{2^{n(n-1) + n(n-2) + n(n-3)}} \right) \right). \]

Proof. Let $C_n=v_1v_2…v_n$ and $v_i^1$, $v_i^2$, …, $v_i^r$ 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 $v^1$, $v^2$, …, $v^r$ be the $r$ hanging vertices of $v$. By the definition of logarithm multiplicative Wiener index, we have

\[ \Pi(I_r(W_n)) = \text{Ln}(\sqrt{2^{n(n-1) + n(n-2) + n(n-3) + n(n-3)}} \cdot \text{Ln} \left( \sqrt{2^{n(n-1) + n(n-2) + n(n-3) + n(n-3)}} \right)). \]

Corollary 2. \[ \Pi(W_n^r) = \text{Ln} \left( \sqrt{2^{n(n-1) + n(n-2) + n(n-3)}} \right). \]

Theorem 3. \[ \Pi(I_r(F_n^r)) = \text{Ln} \left( \sqrt{2^{n(n-1) + n(n-2) + n(n-3) + n(n-3) + n(n-3)}} \cdot \text{Ln} \left( \sqrt{2^{n(n-1) + n(n-2) + n(n-3) + n(n-3) + n(n-3)}} \right) \right). \]

Proof. Let $P_n=v_1v_2…v_n$ and $v_{i,i+1}$ be the adding vertex between $vi$ and $vi+1$. Let $v_i^1$, $v_i^2$, …, $v_i^r$ be the $r$ hanging vertices of $vi$ $(1 \leq i \leq n)$. Let $v_{i,i+1}^1$, $v_{i,i+1}^2$, …, $v_{i,i+1}^r$ 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 $v^1$, $v^2$, …, $v^r$. By virtue of the definition of logarithm multiplicative Wiener index, we get
\[
\Pi(I, \tilde{F}_n) = \ln(2^{n} \prod_{i=1}^{n} d(v, v') \times \prod_{r=1}^{n} d(v, v_r) \times \prod_{j=1}^{n} \prod_{k=1}^{r} d(v, v_{j,k}) \times \prod_{i=1}^{n} d(\tilde{v}_i, v') \times \prod_{i=1}^{n} \prod_{j=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} d(v_i, v_{j,k,l}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} \prod_{m=1}^{r} d(v_i, v_{j,k,l,m})
\]

\[
\prod_{i=1}^{n} \prod_{j=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} d(v_i, v_{j,k,l}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} \prod_{m=1}^{r} d(v_i, v_{j,k,l,m})
\]

\[
= \ln(2^{n} \prod_{i=1}^{n} d(v, v') \times \prod_{r=1}^{n} d(v, v_r) \times \prod_{j=1}^{n} \prod_{k=1}^{r} d(v, v_{j,k}) \times \prod_{i=1}^{n} d(\tilde{v}_i, v') \times \prod_{i=1}^{n} \prod_{j=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} d(v_i, v_{j,k,l}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} \prod_{m=1}^{r} d(v_i, v_{j,k,l,m})
\]

\[
= \ln(2^{n} \prod_{i=1}^{n} d(v, v') \times \prod_{r=1}^{n} d(v, v_r) \times \prod_{j=1}^{n} \prod_{k=1}^{r} d(v, v_{j,k}) \times \prod_{i=1}^{n} d(\tilde{v}_i, v') \times \prod_{i=1}^{n} \prod_{j=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} d(v_i, v_{j,k,l}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} \prod_{m=1}^{r} d(v_i, v_{j,k,l,m})
\]

Corollary 3. \( \Pi(I, \tilde{F}_n) = \ln \sqrt{2^{n} \prod_{i=1}^{n} d(v, v') \times \prod_{r=1}^{n} d(v, v_r) \times \prod_{j=1}^{n} \prod_{k=1}^{r} d(v, v_{j,k}) \times \prod_{i=1}^{n} d(\tilde{v}_i, v') \times \prod_{i=1}^{n} \prod_{j=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} d(v_i, v_{j,k,l}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} \prod_{m=1}^{r} d(v_i, v_{j,k,l,m})}
\]

Corollary 4. \( \Pi(I, \tilde{F}_n) = \ln \sqrt{2^{n} \prod_{i=1}^{n} d(v, v') \times \prod_{r=1}^{n} d(v, v_r) \times \prod_{j=1}^{n} \prod_{k=1}^{r} d(v, v_{j,k}) \times \prod_{i=1}^{n} d(\tilde{v}_i, v') \times \prod_{i=1}^{n} \prod_{j=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} d(v_i, v_{j,k}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} d(v_i, v_{j,k,l}) \times \prod_{i=1}^{n} \prod_{j=1}^{r} \prod_{k=1}^{r} \prod_{l=1}^{r} \prod_{m=1}^{r} d(v_i, v_{j,k,l,m})}
\]
3. Reciprocal Complementary Wiener Index

The notations for special molecular graphs can refer to Theorem 1- Theorem 4.

**Theorem 5.** $RCW(I, (F_n)) = \left(\frac{n^2}{2} - \frac{n}{3} + \frac{1}{2}r^2 + \left(\frac{3}{4}n + \frac{1}{4}r\right) + \left(\frac{2n^2}{3} + \frac{5}{12}\right)\right)$.

**Proof.** By the definition of reciprocal complementary Wiener index, we have

$$
RCW(I, (F_n)) = \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + 
$$

$$
\sum_{i \neq j} \sum_{k \neq l} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \sum_{k \neq l} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \sum_{k \neq l} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \sum_{k \neq l} \frac{1}{1 + D - d(v_i, v_j)} + 
$$

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

$$
\frac{(n-1)(n-2)}{2}r^2 
$$

$$
= \left(\frac{n^2}{2} - \frac{n}{3} + \frac{1}{2}r^2 + \left(\frac{3}{4}n + \frac{1}{4}r\right) + \left(\frac{2n^2}{3} + \frac{5}{12}\right)\right). 
$$

**Corollary 5.** $RCW(F_n) = \frac{n^2 - 3n - 3}{2}$.

**Theorem 6.** $RCW(I, (W_n)) = r^2 \left(\frac{n^2}{2} - \frac{n}{2} + r \left(\frac{11}{12}n + \frac{1}{12}r\right) + \left(\frac{3}{2}n^2 - \frac{1}{2}n\right)\right)$.

**Proof.** By the definition of reciprocal complementary Wiener index, we have

$$
RCW(I, (W_n)) = \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \frac{1}{1 + D - d(v_i, v_j)} + 
$$

$$
\sum_{i \neq j} \sum_{k \neq l} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \sum_{k \neq l} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \sum_{k \neq l} \frac{1}{1 + D - d(v_i, v_j)} + \sum_{i \neq j} \sum_{k \neq l} \frac{1}{1 + D - d(v_i, v_j)} + 
$$

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

$$
\frac{n^2}{2} + \frac{n}{12}r + \left(\frac{11}{12}n + \frac{1}{12}r\right) + \left(\frac{3}{2}n^2 - \frac{1}{2}n\right) 
$$

$$
= r^2 \left(\frac{n^2}{2} - \frac{n}{2} + r \left(\frac{11}{12}n + \frac{1}{12}r\right) + \left(\frac{3}{2}n^2 - \frac{1}{2}n\right)\right). 
$$

**Corollary 6.** $RCW(W_n) = \frac{n^2 + 5n}{2}$.

**Theorem 7.** $RCW(I, (\tilde{F}_n)) = \frac{55n^2 - 98n + 54}{60}r^2 + \frac{85n^2 - 145n + 128}{60}r + \frac{31n^2 - 57n + 44}{60}$.

**Proof.** By virtue of the definition of reciprocal complementary Wiener index, we get
Proof. Theorem 8.

\[
\text{RCW}(I_r(\tilde{F}_n)) = \sum_{i=1}^{n} \frac{1}{1 + \text{d}(v_i, v') + \text{d}(v_i, v''')} + \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_j, v) + \text{d}(v_j, v')} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j) + \text{d}(v_i, v') + \text{d}(v_j, v')} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)}
\]

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

\[
+ \frac{1}{6} \left(2nr + 2n - 1\right) = \frac{1}{5} \left( n - \frac{r^2}{2} + \frac{5n - 7}{2}r^2 + \left(\frac{3n - 2}{2}\right) + \frac{1}{4} \left(3n - 2\right)r^2 + \left(n^2 + 3n - 6\right)r + \left(n - 1\right)(n - 2) \right)
\]

\[
\quad + \frac{1}{3} \left( n^3 - \frac{3n^2}{2} - 3\right) + \frac{2}{3} \left(n - 2\right)(n - 3)r + \frac{1}{2} \left(n - 2\right)(n - 2)r^2 + \left(n - 3\right)(n - 2)r + \frac{\left(n - 2\right)(3n - 2)}{2} = \frac{55n^2 - 98n + 54}{60}r^2 + \frac{85n^2 - 145n + 128}{60}r + \frac{31n^2 - 57n + 44}{60}.
\]

Corollary 7. \(\text{RCW}(\tilde{F}_n) = \frac{14n^2 - 36n + 33}{12} \). Theorem 8. \(\text{RCW}(I_r(\tilde{W}_n)) = \frac{70n^2 - 63n}{60}r^2 + \frac{85n^2 - 69n + 10}{60}r + \frac{31n^2 - 12n + 12}{60} \).

Proof. In view of the definition of reciprocal complementary Wiener index, we deduce

\[
\text{RCW}(I_r(\tilde{W}_n)) = \sum_{i=1}^{n} \frac{1}{1 + \text{d}(v_i, v') + \text{d}(v_i, v'')} + \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_j, v) + \text{d}(v_j, v')} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j) + \text{d}(v_i, v') + \text{d}(v_j, v')} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j) + \text{d}(v_i, v_k)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j) + \text{d}(v_i, v_k)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j) + \text{d}(v_i, v_k)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j) + \text{d}(v_i, v_k)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j) + \text{d}(v_i, v_k)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j) + \text{d}(v_i, v_k)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{1 + \text{d}(v_i, v_j)}.
\]
\[
\sum_{i=1}^{n} \sum_{j=1}^{n} \frac{1}{D(v_i, v_j)} + \sum_{k=1}^{n} \sum_{t=1}^{n} \frac{1}{D(v_k, v_t)} = \frac{1}{6} (r(2n+1)+3n) + \frac{1}{5} (nr^2 + 3nr + \frac{n^2}{2} + 3n + 1) + \frac{1}{4} (3nr^2 + n(n+3)r + n(n-2)) \\
+ \frac{1}{3} \left( \frac{n^3}{2} + \frac{3n}{2} \right) r^2 + 2(n-2)nr + \frac{n(n-3)}{2} r \right) + \frac{1}{2} \left( (n-2)nr^2 + (n-3)nr + \frac{n(n-3)}{2} r^2 \\
= 70n^2 - 63n - 60 \frac{r^2}{r^2} + \frac{85n^2 - 69n + 10}{60} r^2 + \frac{3ln^2 - 12n + 12}{60} r.
\]

Corollary 8. \( RCW(W) = \frac{14n^2 - 24n + 13}{12} \)

4. Conclusion

In this paper, we present the logarithmic multiplicative Wiener index and reciprocal complementary Wiener index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their \( r \)-corona molecular graphs. The results obtained in our paper illustrate the promising application prospects for chemistry and pharmacy science.

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