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Edge Wiener Index of Gear Related Molecular Graphs and Their *r*-Corona Molecular Graphs

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Abstract

Chemical compounds and drugs are often modelled as graphs (for example, Polyhex Nanotubes and Dendrimer Nanostar) 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. The edge Wiener index of a graph is defined as the sum of the distances between all pairs of edges, and it has been found extensive applications in chemistry. In this paper, we determine the edge Wiener index of gear fan graph, gear wheel graph and their *r*-corona graphs.

Keywords

Organic Molecules, Edge Wiener Index, Fan Graph, Wheel Graph, Gear Fan Graph, Gear Wheel Graph, *r*-Corona Graph

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1. Introduction

Wiener index, Hyper-Wiener index and edge Wiener index are introduced to reflect certain structural features of organic molecules. We denote P_n and C_n are path and cycle with n vertices. The graph $F_n=\{v\}\vee P_n$ is called a fan graph and the graph $W_n=\{v\}\vee C_n$ is called a wheel graph. Graph $I_r(G)$ is called r- crown graph of G which splicing r hang edges for every vertex in G. 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 $\tilde{F}_n$. 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 $\tilde{W}_n$.

The (molecular) 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. The Hyper-wiener index is defined as

$$WW(G)=\frac{1}{2}\sum_{\{u,v\}\subseteq V(G)}\{d(u,v)+d(u,v)^2\}.$$

Several papers contributed to determine the Wiener index and Hyper-wiener index of special graphs. Yan et al., [1] presented the graphs which minimize the Hyper-Wiener index among all graphs with given chromatic number and clique number and the graphs which maximum the Hyper-Wiener index among all graphs with given chromatic number and clique number. More results 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].

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Then the edge-Wiener index of G is defined as the sum of the distances (in the line graph) between all pairs of edges of G, i.e.,

$$W_e(G)=\sum_{\{e,f\}\subseteq E(G)} d(e,f),$$

where the distance between two edges is the distance between the corresponding vertices in the line graph of G.

Buckley [11] proved that $W_e(T)=W(T)-\binom{n}{2}$ for a tree with order n. Gutman [12] presented that if G is a connected graph of order n and size q, then $W_e(G) \geq W(G)-n(n-1)+\frac{1}{2}q(q+1)$. Gutman and Pavlovic [13] showed that if G is a connected unicyclic graph of order n, then $W_e(G)\leq W(G)$, with equality if and only if $G\cong C_n$. Recently, Dankelmanna et al., [14] verified that the asymptotically sharp upper bound $W_e(G) \leq \frac{2^5}{5^5}n^5+O(n^{\frac{9}{2}})$ for graphs of order n.

In this paper, we present the edge wiener index of $I_r(F_n)$ and $I_r(W_n)$ first; then, the edge wiener index of gear fan graph and gear wheel graph are determined; at last, the edge wiener index of $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$ are derived.

2. Main Results and Proof

Theorem 1. $W_e(I_r(F_n))$ = $r^2(\frac{3}{2}n^2+\frac{3}{2})$ + $r(5n^2-\frac{15}{2}n+\frac{11}{2})$ + $(4n^2-12n+12)$.

Proof. Let Pn=v1v2…vn and the r hanging vertices of vi be v_i^1, v_i^2,…, v_i^r (1≤i≤n). Let v be a vertex in Fn beside Pn, and the r hanging vertices of v be v^1, v^2, …, v^r.

By the definition of edge Wiener index, we have

$$\begin{aligned}W_e(I_r(F_n))&=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}d(vv^i,vv^j)+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v_iv_i^j,v_iv_i^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v_iv_i^k,v_jv_j^t)+\sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r}d(vv^i,v_jv_j^k)\\&+\sum_{i=1}^{r}\sum_{j=1}^{n}d(vv^i,vv_j)+\sum_{i=1}^{r}\sum_{j=1}^{n-1}d(vv^i,v_jv_{j+1})+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r}d(vv_i,v_jv_j^k)+\sum_{i=1}^{n-1}\sum_{j=1}^{n}\sum_{k=1}^{r}d(v_iv_{i+1},v_jv_j^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(vv_i,vv_j)\\&+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}d(v_iv_{i+1},v_jv_{j+1})+\sum_{i=1}^{n}\sum_{j=1}^{n-1}d(vv_i,v_jv_{j+1})\\&=\frac{r(r-1)}{2}+\frac{nr(r-1)}{2}+r^2(\frac{3}{2}n^2-\frac{5n}{2}+1)+2nr^2+rn+2r(n-1)+r(2n^2-n)+r(3n^2-9n+8)+\frac{n(n-1)}{2}\\&+(\frac{3}{2}n^2-\frac{15}{2}n+10)+(2n^2-4n+2)\\&=r^2(\frac{3}{2}n^2+\frac{3}{2})+r(5n^2-\frac{15}{2}n+\frac{11}{2})+(4n^2-12n+12).\end{aligned}$$

Corollary 1. $W_e(F_n)=4n^2-12n+12$.

Theorem 2. $W_e(I_r(W_n))=r^2(\frac{3}{2}n^2+\frac{1}{2})+r(5n^2-\frac{9}{2}n-\frac{1}{2})+(4n^2-7n)$.

Proof. Let $C_n=v_1v_2\ldots v_n$ 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. We denote $v_nv_{n+1}=v_nv_1$.

By the definition of edge Wiener index, we have

$$\begin{aligned}W_e(I_r(W_n))&=\sum_{i=1}^{r-1}\sum_{j=i+1}^{r}d(vv^i,vv^j)+\sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r}d(v_iv_i^j,v_iv_i^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r}d(v_iv_i^k,v_jv_j^t)\ \sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r}d(vv^i,v_jv_j^k)\\&+\sum_{i=1}^{r}\sum_{j=1}^{n}d(vv^i,vv_j)+\sum_{i=1}^{r}\sum_{j=1}^{n}d(vv^i,v_jv_{j+1})+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r}d(vv_i,v_jv_j^k)+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r}d(v_iv_{i+1},v_jv_j^k)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}d(vv_i,vv_j)\end{aligned}$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_iv_{i+1},v_jv_{j+1})+\sum_{i=1}^{n}\sum_{j=1}^{n} d(vv_i,v_jv_{j+1})$$

$$=\frac{r(r-1)}{2}+\frac{nr(r-1)}{2}+r^2(\frac{3}{2}n^2-\frac{5}{2}n)+2nr^2+rn+2rn+r(2n^2-n)+r(3n^2-6n)+\frac{n(n-1)}{2}+(\frac{3}{2}n^2-\frac{9}{2}n)$$

$$+(2n^2-2n)$$

$$=r^2(\frac{3}{2}n^2+\frac{1}{2})+r(5n^2-\frac{9}{2}n-\frac{1}{2})+(4n^2-7n).$$

Corollary 2. $W_e(W_n)=4n^2-7n$.

Theorem 3. $W_e(\tilde{F}_n)=\frac{21}{2}n^2-\frac{59}{2}n+19$.

Proof. Let $P_n=v_1v_2\ldots v_n$ and $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. Let v be a vertex in F_n beside P_n. By virtue of the definition of edge Wiener index, we get

$$W_e(\tilde{F}_n)=\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(vv_i,vv_j)+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_iv_{i,i+1},v_jv_{j.j+1})+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_{i,i+1}v_{i+1},v_{j.j+1}v_{j+1})+\sum_{i=1}^{n-1}\sum_{j=1}^{n-1} d(v_iv_{i,i+1},v_{j.j+1}v_{j+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n-1} d(vv_i,v_jv_{j,j+1})+\sum_{i=1}^{n}\sum_{j=1}^{n-1} d(vv_i,v_{j,j+1}v_{j+1})$$

$$=\frac{n(n-1)}{2}+(\frac{3}{2}n^2-\frac{11}{2}n+5)+(\frac{3}{2}n^2-\frac{11}{2}n+5)+(3n^2-12n+9)+(2n^2-3n)+(2n^2-3n)$$

$$=\frac{21}{2}n^2-\frac{59}{2}n+19.$$

Theorem 4. $W_e(\tilde{W}_n)=\frac{21}{2}n^2-\frac{23}{2}n$.

Proof. Let $C_n=v_1v_2\ldots v_n$ and v be a vertex in W_n beside C_n. Let $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. Let $v_{n.n+1}=v_{n.1}$, $v_{n+1}=v_1$. In view of the definition of edge Wiener index, we deduce

$$W_e(\tilde{W}_n)=\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(vv_i,vv_j)+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_iv_{i,i+1},v_jv_{j.j+1})+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_{i,i+1}v_{i+1},v_{j.j+1}v_{j+1})+\sum_{i=1}^{n}\sum_{j=1}^{n} d(v_iv_{i,i+1},v_{j.j+1}v_{j+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n} d(vv_i,v_jv_{j,j+1})+\sum_{i=1}^{n}\sum_{j=1}^{n} d(vv_i,v_{j,j+1}v_{j+1})$$

$$=\frac{n(n-1)}{2}+(\frac{3}{2}n^2-\frac{5}{2}n)+(\frac{3}{2}n^2-\frac{5}{2}n)+(3n^2-4n)+(2n^2-n)+(2n^2-n)$$

$$=\frac{21}{2}n^2-\frac{23}{2}n.$$

Theorem 5. $W_e(I_r(\tilde{F}_n))=r^2(8n^2-14n+11)+r(19n^2-38n+30)+(\frac{21}{2}n^2-\frac{59}{2}n+19)$.

Proof. Let $P_n=v_1v_2\ldots v_n$ and $v_{i,i+1}$ be the adding vertex between v_i and v_{i+1}. Let v_i^1, v_i^2,…, v_i^r be the r hanging vertices of vi ($1\le i\le n$). Let $v_{i,i+1}^1$, $v_{i,i+1}^2$,…, $v_{i,i+1}^r$ be the r hanging vertices of $v_{i,i+1}$ ($1\le i\le n$-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 edge Wiener index, we get

$$W_e(I_r(\tilde{F}_n)) = \{\sum_{i=1}^{r-1}\sum_{j=i+1}^{r} d(vv^i, vv^j) + \sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_iv_i^j, v_iv_i^k) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_iv_i^k, v_jv_j^t) + \sum_{i=1}^{n-1}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_{i,i+1}v_{i,i+1}^j, v_{i,i+1}v_{i,i+1}^k)$$

$$+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_{i,i+1}v_{i,i+1}^k, v_{j,j+1}v_{j,j+1}^t) + \sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r} d(vv^i, v_jv_j^k) + \sum_{i=1}^{r}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(vv^i, v_{j,j+1}v_{j,j+1}^k)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n-1}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_iv_i^k, v_{j,j+1}v_{j,j+1}^t) + \sum_{i=1}^{r}\sum_{j=1}^{n} d(vv^i, vv_j) + \sum_{i=1}^{r}\sum_{j=1}^{n-1} d(vv^i, v_jv_{j,j+1}) + \sum_{i=1}^{r}\sum_{j=1}^{n-1} d(vv^i, v_{j,j+1}v_{j+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r} d(vv_i, v_jv_j^k) + \sum_{i=1}^{n-1}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v_iv_{i,i+1}, v_jv_j^k) + \sum_{i=1}^{n-1}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v_{i,i+1}v_{i+1}, v_jv_j^k) + \sum_{i=1}^{n}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(vv_i, v_{j,j+1}v_{j,j+1}^k)$$

$$+\sum_{i=1}^{n-1}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v_iv_{i,i+1}, v_{j,j+1}v_{j,j+1}^k) + \sum_{i=1}^{n-1}\sum_{j=1}^{n-1}\sum_{k=1}^{r} d(v_{i,i+1}v_{i+1}, v_{j,j+1}v_{j,j+1}^k)\} + \{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(vv_i, vv_j) + \sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_iv_{i,i+1}, v_jv_{j.j+1})$$

$$+\sum_{i=1}^{n-2}\sum_{j=i+1}^{n-1} d(v_{i,i+1}v_{i+1}, v_{j.j+1}v_{j+1}) + \sum_{i=1}^{n-1}\sum_{j=1}^{n-1} d(v_iv_{i,i+1}, v_{j.j+1}v_{j+1}) + \sum_{i=1}^{n}\sum_{j=1}^{n-1} d(vv_i, v_jv_{j,j+1}) + \sum_{i=1}^{n}\sum_{j=1}^{n-1} d(vv_i, v_{j,j+1}v_{j+1})\}$$

$$=\{\frac{r(r-1)}{2} + \frac{nr(r-1)}{2} + r^2(\frac{3}{2}n^2 - \frac{5}{2}n + 1) + \frac{(n-1)r(r-1)}{2} + r^2(\frac{5}{2}n^2 - \frac{19}{2}n + 9) + 2r^2n + 3r^2(n-1) + 4r^2(n^2 - 2n + 1)$$

$$+rn + 2r(n-1) + 2r(n-1) + r(2n^2 - n) + r(3n^2 - 6n + 3) + r(3n^2 - 6n + 3) + r(3n^2 - 5n + 2) + r(4n^2 - 12n + 13)$$

$$+r(4n^2 - 12n + 13)\} + \{\frac{n(n-1)}{2} + (\frac{3}{2}n^2 - \frac{11}{2}n + 5) + (\frac{3}{2}n^2 - \frac{11}{2}n + 5) + (3n^2 - 12n + 9) + (2n^2 - 3n) + (2n^2 - 3n)\}$$

$$= r^2(8n^2 - 14n + 11) + r(19n^2 - 38n + 30) + (\frac{21}{2}n^2 - \frac{59}{2}n + 19).$$

Theorem 6. $W_e(I_r(\tilde{W}_n)) = r^2(8n^2 - 4n + \frac{1}{2}) + r(19n^2 - 17n - \frac{1}{2}) + (\frac{21}{2}n^2 - \frac{23}{2}n)$.

Proof. Let $C_n=v_1v_2\ldots v_n$ 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, …, v^r. be the r hanging vertices of v and v_i^1, v_i^2,…, v_i^r be the r hanging vertices of v_i ($1 \le i \le n$). Let $v_{n,n+1} = v_{1,n}$ and $v_{i,i+1}^1$, $v_{i,i+1}^2$,…, $v_{i,i+1}^r$ be the r hanging vertices of $v_{i,i+1}$ ($1 \le i \le n$). Let $v_{n.n+1} = v_{n.1}$, $v_{n+1} = v_1$. In view of the definition of edge Wiener index, we deduce

$$W_e(I_r(\tilde{W}_n)) = \{\sum_{i=1}^{r-1}\sum_{j=i+1}^{r} d(vv^i, vv^j) + \sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_iv_i^j, v_iv_i^k) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_iv_i^k, v_jv_j^t) + \sum_{i=1}^{n}\sum_{j=1}^{r-1}\sum_{k=j+1}^{r} d(v_{i,i+1}v_{i,i+1}^j, v_{i,i+1}v_{i,i+1}^k)$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_{i,i+1}v_{i,i+1}^k, v_{j,j+1}v_{j,j+1}^t) + \sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r} d(vv^i, v_jv_j^k) + \sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r} d(vv^i, v_{j,j+1}v_{j,j+1}^k)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r}\sum_{t=1}^{r} d(v_iv_i^k, v_{j,j+1}v_{j,j+1}^t) + \sum_{i=1}^{r}\sum_{j=1}^{n} d(vv^i, vv_j) + \sum_{i=1}^{r}\sum_{j=1}^{n} d(vv^i, v_jv_{j,j+1}) + \sum_{i=1}^{r}\sum_{j=1}^{n} d(vv^i, v_{j,j+1}v_{j+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r} d(vv_i, v_jv_j^k) + \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v_iv_{i,i+1}, v_jv_j^k) + \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v_{i,i+1}v_{i+1}, v_jv_j^k) + \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r} d(vv_i, v_{j,j+1}v_{j,j+1}^k)$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v_iv_{i,i+1}, v_{j,j+1}v_{j,j+1}^k) + \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{k=1}^{r} d(v_{i,i+1}v_{i+1}, v_{j,j+1}v_{j,j+1}^k)\} + \{\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(vv_i, vv_j) + \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_iv_{i,i+1}, v_jv_{j,j+1})$$

$$+\sum_{i=1}^{n-1}\sum_{j=i+1}^{n} d(v_{i,i+1}v_{i+1}, v_{j,j+1}v_{j+1}) + \sum_{i=1}^{n}\sum_{j=1}^{n} d(v_i v_{i,i+1}, v_{j,j+1}v_{j+1}) + \sum_{i=1}^{n}\sum_{j=1}^{n} d(vv_i, v_j v_{j,j+1}) + \sum_{i=1}^{n}\sum_{j=1}^{n} d(vv_i, v_{j,j+1}v_{j+1}) \}$$

$$=\{ \frac{r(r-1)}{2} + \frac{nr(r-1)}{2} + r^2(\frac{3}{2}n^2 - \frac{3}{2}n) + \frac{nr(r-1)}{2} + r^2(\frac{5}{2}n^2 - \frac{9}{2}n) + 2r^2 n + 3r^2 n + 4r^2(n^2-n) + rn + 2rn + 2rn$$

$$+ r(2n^2-n) + r(3n^2-3n) + r(3n^2-3n) + r(3n^2-2n) + r(4n^2-6n) + r(4n^2-6n) \} + \{ \frac{n(n-1)}{2} + (\frac{3}{2}n^2 - \frac{5}{2}n)$$

$$+ (\frac{3}{2}n^2 - \frac{5}{2}n) + (3n^2-4n) + (2n^2-n) + (2n^2-n) \}$$

$$= r^2(8n^2 - 4n + \frac{1}{2}) + r(19n^2 - 17n - \frac{1}{2}) + (\frac{21}{2}n^2 - \frac{23}{2}n) .$$

3. Conclusion

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 edge Wiener index, has been shown to be strongly correlated to various chemical properties of the compounds. 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 edge Wiener index of these special structural features of organic molecules.

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