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Geometric-arithmetic Index and Zagreb Indices of Certain Special Molecular Graphs

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Abstract: In this paper, we determine the Geometric-arithmetic indexand Zagreb indicesof fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their *r*-corona molecular graphs.

Keywords: Chemical graph theory, Geometric-arithmetic index, Zagreb index, Fan molecular graph, Wheel molecular graph, Gear fan moleculargraph, Gear wheel moleculargraph, *r*-corona moleculargraph

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1. INTRODUCTION

Wiener index,edge Wiener index, Hyper-wiener 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 of special molecular graphs (See Yan et al., [1] and [2], Gao and Shi [3] for more detail). LetP_n and $C_n$be path and cycle with n vertices. The molecular graph $F_n=\{v\}\vee P_n$is called a fan molecular graph and the molecular graph $W_n=\{v\}\vee C_n$is called a wheel molecular graph. Molecular graph $I_r(G)$ is called r- crown molecular 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 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 $\tilde{W}_n$.

By considering the degrees of vertices in G, Vukicevic and Furtula [4]developed the Geometric-arithmetic index, shortly GA index, which is defined by

$$GA(G)=\sum_{uv\in E(G)}\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)},$$

where$d(u)$ and $d(v)$ are the degrees of u and v, respectively.

The (first and second) Zagreb indices have been introduced by Gutman and Trinajstic[5] as the form

$$M_1(G)=\sum_{v\in V(G)}(d(v))^2,$$

and

$$M_2(G)=\sum_{uv\in E(G)}d(u)d(v).$$

On the other hand, for a moleculargraph G, the modified second Zagreb index $M_2^*(G)$ is defined as

$$M_2^*(G)=\sum_{uv\in E(G)}\frac{1}{d(u)d(v)}.$$

Several papers contributed on determining the Zagreb indices of special molecular graphs can refer to [6-10].

In this paper, we present the Geometric-arithmetic index of $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$. Also, the Zagreb indices of $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$ are derived.

2. GEOMETRIC-ARITHMETICINDEX

Theorem 1. $GA(I_r(F_n))=\frac{2r\sqrt{n+r}}{n+r+1}+\frac{4\sqrt{(n+r)(2+r)}}{n+2r+2}+\frac{2(n-2)\sqrt{(n+r)(3+r)}}{n+2r+3}$

$+\frac{4\sqrt{(2+r)(3+r)}}{2r+5}+\frac{(n-3)\sqrt{(3+r)(3+r)}}{r+3}+\frac{4r\sqrt{2+r}}{r+3}+\frac{2(n-2)r\sqrt{3+r}}{r+4}.$

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,…, v_i^r ($1\le i\le n$). 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 Geometric-arithmetic index, we have

$$GA(I_r(F_n))=\sum_{i=1}^{r}\frac{2\sqrt{d(v)d(v^i)}}{d(v)+d(v^i)}+\sum_{i=1}^{n}\frac{2\sqrt{d(v)d(v_i)}}{d(v)+d(v_i)}+\sum_{i=1}^{n-1}\frac{2\sqrt{d(v_i)d(v_{i+1})}}{d(v_i)+d(v_{i+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r}\frac{2\sqrt{d(v_i)d(v_i^j)}}{d(v_i)+d(v_i^j)}$$

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

$$+\left(\frac{4\sqrt{(2+r)(3+r)}}{2r+5}+\frac{(n-3)\sqrt{(3+r)(3+r)}}{r+3}\right)+\left(\frac{4r\sqrt{2+r}}{r+3}+\frac{2(n-2)r\sqrt{3+r}}{r+4}\right).\ \square$$

Corollary 1. $GA(F_n)=\frac{4\sqrt{2n}}{n+2}+\frac{2(n-2)\sqrt{3n}}{n+3}+\frac{4\sqrt{6}}{5}+n-3$.

Theorem 2. $GA(I_r(W_n))=\frac{2r\sqrt{n+r}}{n+r+1}+\frac{2n\sqrt{(n+r)(3+r)}}{n+2r+3}+\frac{n\sqrt{(3+r)(3+r)}}{r+3}+\frac{2nr\sqrt{3+r}}{r+4}$.

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 $v_i(1\le i\le n)$. 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 Geometric-arithmetic index, we have

$$GA(I_r(W_n))=\sum_{i=1}^{r}\frac{2\sqrt{d(v)d(v^i)}}{d(v)+d(v^i)}+\sum_{i=1}^{n}\frac{2\sqrt{d(v)d(v_i)}}{d(v)+d(v_i)}+\sum_{i=1}^{n}\frac{2\sqrt{d(v_i)d(v_{i+1})}}{d(v_i)+d(v_{i+1})}+\sum_{i=1}^{n}\sum_{j=1}^{r}\frac{2\sqrt{d(v_i)d(v_i^j)}}{d(v_i)+d(v_i^j)}$$

$$=\frac{2r\sqrt{n+r}}{n+r+1}+\frac{2n\sqrt{(n+r)(3+r)}}{n+2r+3}+\frac{n\sqrt{(3+r)(3+r)}}{r+3}+\frac{2nr\sqrt{3+r}}{r+4}.\ \square$$

Corollary 2. $GA(W_n)=\frac{2n\sqrt{3n}}{n+3}+n$.

Theorem 3. $GA(I_r(\tilde{F}_n))=\frac{2r\sqrt{n+r}}{n+r+1}+\frac{4\sqrt{(n+r)(2+r)}}{n+2r+2}+\frac{2(n-2)\sqrt{(n+r)(3+r)}}{n+2r+3}$

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

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 $v_i(1\le i\le n)$. 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 Geometric-arithmetic index, we get

$$GA(I_r(\tilde{F}_n)) = \sum_{i=1}^{r}\frac{2\sqrt{d(v)d(v^i)}}{d(v)+d(v^i)} + \sum_{i=1}^{n}\frac{2\sqrt{d(v)d(v_i)}}{d(v)+d(v_i)} + \sum_{i=1}^{n}\sum_{j=1}^{r}\frac{2\sqrt{d(v_i)d(v_i^j)}}{d(v_i)+d(v_i^j)} + \sum_{i=1}^{n-1}\frac{2\sqrt{d(v_i)d(v_{i,i+1})}}{d(v_i)+d(v_{i,i+1})} +$$

$$\sum_{i=1}^{n-1}\frac{2\sqrt{d(v_{i,i+1})d(v_{i+1})}}{d(v_{i,i+1})+d(v_{i+1})} + \sum_{i=1}^{n-1}\sum_{j=1}^{r}\frac{2\sqrt{d(v_{i,i+1})d(v^j_{i,i+1})}}{d(v_{i,i+1})+d(v^j_{i,i+1})}$$

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

$$+\left(\frac{4r\sqrt{2+r}}{r+3} + \frac{2(n-2)r\sqrt{3+r}}{r+4}\right) + \left(\frac{\sqrt{(2+r)(2+r)}}{r+2} + \frac{2(n-2)\sqrt{(3+r)(2+r)}}{2r+5}\right)$$

$$+\left(\frac{\sqrt{(2+r)(2+r)}}{r+2} + \frac{2(n-2)\sqrt{(3+r)(2+r)}}{2r+5}\right) + \frac{2(n-1)r\sqrt{2+r}}{r+3}.$$

□ **Corollary3.** $GA(\tilde{F}_n) = \frac{4\sqrt{2n}}{n+2} + \frac{2(n-2)\sqrt{3n}}{n+3} + \frac{4(n-2)\sqrt{6}+10}{5}$.

Theorem4. $GA(I_r(\tilde{W}_n)) = \frac{2r\sqrt{n+r}}{n+r+1} + \frac{2n\sqrt{(n+r)(3+r)}}{n+2r+3} + \frac{2nr\sqrt{3+r}}{r+4} + \frac{4n\sqrt{(3+r)(2+r)}}{2r+5} + \frac{2nr\sqrt{2+r}}{r+3}$.

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 $v^1_{i,i+1}$, $v^2_{i,i+1}$,…, $v^r_{i,i+1}$ be the r hanging vertices of $v_{i,i+1}$ ($1\le i\le n$). In view of the definition of Geometric-arithmetic index, we deduce

$$GA(I_r(\tilde{W}_n)) = \sum_{i=1}^{r}\frac{2\sqrt{d(v)d(v^i)}}{d(v)+d(v^i)} + \sum_{i=1}^{n}\frac{2\sqrt{d(v)d(v_i)}}{d(v)+d(v_i)} + \sum_{i=1}^{n}\sum_{j=1}^{r}\frac{2\sqrt{d(v_i)d(v_i^j)}}{d(v_i)+d(v_i^j)} + \sum_{i=1}^{n}\frac{2\sqrt{d(v_i)d(v_{i,i+1})}}{d(v_i)+d(v_{i,i+1})} +$$

$$\sum_{i=1}^{n}\frac{2\sqrt{d(v_{i,i+1})d(v_{i+1})}}{d(v_{i,i+1})+d(v_{i+1})} + \sum_{i=1}^{n}\sum_{j=1}^{r}\frac{2\sqrt{d(v_{i,i+1})d(v^j_{i,i+1})}}{d(v_{i,i+1})+d(v^j_{i,i+1})}$$

$$= \frac{2r\sqrt{n+r}}{n+r+1} + \frac{2n\sqrt{(n+r)(3+r)}}{n+2r+3} + \frac{2nr\sqrt{3+r}}{r+4} + \frac{2n\sqrt{(3+r)(2+r)}}{2r+5} + \frac{2n\sqrt{(3+r)(2+r)}}{2r+5} + \frac{2nr\sqrt{2+r}}{r+3}.$$ □

Corollary 4. $GA(\tilde{W}_n) = \frac{2n\sqrt{3n}}{n+3} + \frac{4n\sqrt{6}}{5}$.

3. ZAGREB INDICES

Using the notations defined in above section, and combining with the definitions of Zagreb indices, we get the following computational formulas.

$$M_1(I_r(F_n)) = (d(v))^2 + \sum_{i=1}^{r}(d(v^i))^2 + \sum_{i=1}^{n}(d(v_i))^2 + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i^j))^2$$

$$= (n+r)^2 + r + 2(2+r)^2 + (n-2)(3+r)^2 + nr$$

$$= r^2(n+1) + r(9n-3) + n^2 + 9n - 10.$$

$$M_1(F_n) = n^2 + 9n - 10.$$

$$M_1(I_r(W_n)) = (d(v))^2 + \sum_{i=1}^{r}(d(v^i))^2 + \sum_{i=1}^{n}(d(v_i))^2 + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i^j))^2$$

$$= (n+r)^2 + r + n(3+r)^2 + nr$$

$$= r^2(n+1) + r(9n+1) + n^2 + 9n.$$

$$M_1(W_n) = n^2 + 9n.$$

$$M_1(I_r(\tilde{F}_n)) = (d(v))^2 + \sum_{i=1}^{r}(d(v^i))^2 + \sum_{i=1}^{n}(d(v_i))^2 + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i^j))^2 + \sum_{i=1}^{n-1}(d(v_{i,i+1}))^2$$

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

$$= (n+r)^2 + r + 2(2+r)^2 + (n-2)(3+r)^2 + nr + (n-1)(2+r)^2 + r(n-1)$$

$$= 2nr^2 + r(14n-8) + n^2 + 13n - 14.$$

$$M_1(\tilde{F}_n) = n^2 + 13n - 14.$$

$$M_1(I_r(\tilde{W}_n)) = (d(v))^2 + \sum_{i=1}^{r}(d(v^i))^2 + \sum_{i=1}^{n}(d(v_i))^2 + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i^j))^2 + \sum_{i=1}^{n}(d(v_{i,i+1}))^2$$

$$+ \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_{i,i+1}^j))^2$$

$$= (n+r)^2 + r + n(3+r)^2 + nr + n(2+r)^2 + nr$$

$$= r^2(2n+1) + r(14n+1) + n^2 + 13n.$$

$$M_1(\tilde{W}_n) = n^2 + 13n.$$

$$M_2(I_r(F_n)) = \sum_{i=1}^{r} d(v)d(v^i) + \sum_{i=1}^{n} d(v)d(v_i) + \sum_{i=1}^{n-1} d(v_i)d(v_{i+1}) + \sum_{i=1}^{n}\sum_{j=1}^{r} d(v_i)d(v_i^j)$$

$$=r(n+r)+(2(n+r)(2+r)+(n-2)(n+r)(3+r))+(2(2+r)(3+r)+(n-3)(3+r)(3+r))$$

$$+(2r(2+r)+(n-2)r(3+r))$$

$$=3r^2n+r(n^2+13n-12)+3n^2+7n-15.$$

$$M_2(F_n)=3n^2+7n-15.$$

$$M_2(I_r(W_n))=\sum_{i=1}^{r}d(v)d(v^i)+\sum_{i=1}^{n}d(v)d(v_i)+\sum_{i=1}^{n}d(v_i)d(v_{i+1})+\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v_i^j)$$

$$=r(n+r)+n(n+r)(3+r)+n(3+r)(3+r)+nr(3+r).$$

$$=r^2(3n+1)+r(n^2+13n)+3n^2+9n$$

$$M_2(W_n)=3n^2+9n.$$

$$M_2(I_r(\tilde{F}_n)) = \sum_{i=1}^{r}d(v)d(v^i) + \sum_{i=1}^{n}d(v)d(v_i) + \sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v_i^j) + \sum_{i=1}^{n-1}d(v_i)d(v_{i,i+1}) + \sum_{i=1}^{n-1}d(v_{i,i+1})d(v_{i+1}) +$$

$$\sum_{i=1}^{n-1}\sum_{j=1}^{r}d(v_{i,i+1})d(v^j_{i,i+1})$$

$$= r(n+r) + (2(n+r)(2+r)+(n-2)(n+r)(3+r)) + (2r(2+r)+(n-2)r(3+r)) +$$

$$((2+r)(2+r)+(n-2)(3+r)(2+r))+((2+r)(2+r)+(n-2)(3+r)(2+r))$$

$$+(n-1)r(2+r)$$

$$=r^2(5n-3)+r(n^2+19n-18)+3n^2+10n-16.$$

$$M_2(\tilde{F}_n)=3n^2+10n-16.$$

$$M_2(I_r(\tilde{W}_n)) = \sum_{i=1}^{r}d(v)d(v^i) + \sum_{i=1}^{n}d(v)d(v_i) + \sum_{i=1}^{n}\sum_{j=1}^{r}d(v_i)d(v_i^j) + \sum_{i=1}^{n}d(v_i)d(v_{i,i+1}) + \sum_{i=1}^{n}d(v_{i,i+1})d(v_{i+1}) +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}d(v_{i,i+1})d(v^j_{i,i+1})$$

$$=r(n+r)+n(n+r)(3+r)+nr(3+r)+n(3+r)(2+r)+n(3+r)(2+r)+nr(2+r)$$

$$=r^2(5n+1)+r(n^2+19n)+3n^2+12n$$

$$M_2(\tilde{W}_n)=3n^2+12n.$$

$$M_2^*(I_r(F_n)) = \sum_{i=1}^{r}(d(v)d(v^i))^{-1} + \sum_{i=1}^{n}(d(v)d(v_i))^{-1} + \sum_{i=1}^{n-1}(d(v_i)d(v_{i+1}))^{-1} + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)d(v_i^j))^{-1}$$

$$= \frac{r}{n+r} + \frac{2}{(n+r)(2+r)} + \frac{n-2}{(n+r)(3+r)} + \frac{2}{(2+r)(3+r)} + \frac{n-3}{(3+r)(3+r)}$$

$$+ \frac{2r}{2+r} + \frac{(n-2)r}{3+r}.$$

$$M_2^*(F_n) = \frac{1}{n} + \frac{n-2}{3n} + \frac{1}{3} + \frac{n-3}{9}.$$

$$M_2^*(I_r(W_n)) = \sum_{i=1}^{r}(d(v)d(v^i))^{-1} + \sum_{i=1}^{n}(d(v)d(v_i))^{-1} + \sum_{i=1}^{n}(d(v_i)d(v_{i+1}))^{-1} + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)d(v_i^j))^{-1}$$

$$= \frac{r}{n+r} + \frac{n}{(n+r)(3+r)} + \frac{n}{(3+r)(3+r)} + \frac{nr}{3+r}.$$

$$M_2^*(W_n) = \frac{1}{3} + \frac{n}{9}.$$

$$M_2^*(I_r(\tilde{F}_n)) = \sum_{i=1}^{r}(d(v)d(v^i))^{-1} + \sum_{i=1}^{n}(d(v)d(v_i))^{-1} + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)d(v_i^j))^{-1} + \sum_{i=1}^{n-1}(d(v_i)d(v_{i,i+1}))^{-1} +$$

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

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

$$M_2^*(\tilde{F}_n) = \frac{1}{n} + \frac{n-2}{3n} + \frac{1}{2} + \frac{n-2}{3}.$$

$$M_2^*(I_r(\tilde{W}_n)) = \sum_{i=1}^{r}(d(v)d(v^i))^{-1} + \sum_{i=1}^{n}(d(v)d(v_i))^{-1} + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)d(v_i^j))^{-1} + \sum_{i=1}^{n}(d(v_i)d(v_{i,i+1}))^{-1} +$$

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

$$= \frac{r}{n+r} + \frac{n}{(n+r)(3+r)} + \frac{nr}{3+r} + \frac{2n}{(3+r)(2+r)} + \frac{nr}{2+r}.$$

$$M_2^*(\tilde{W}_n) = \frac{n+1}{3}.$$

4. CONCLUSION

In this paper, we determine the Geometric-arithmetic index and Zagreb indices of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their *r*-corona molecular graphs.

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