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General randic index and geometrix-arithmetic related indices of certain special molecular graphs

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ABSTRACT

Some chemical indices have been invented in theoretical chemistry, such as Randic index and geometric-arithmetic index. In this paper, by virtue of strict mathematical deduction, we present the general Randic index, general geometric-arithmetic index and third geometric-arithmetic index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs.

KEYWORDS

Theoretical chemistry; Molecular graph; General randic index; General geometric-arithmetic index; Third geometric-arithmetic index.

INTRODUCTION

Geometric-arithmetic index, Randic index and other chemical indices are introduced to reflect certain structural features of organic molecules (See Yan et al.,[1], Gao and Shi [2], Gao and Wang [3], and Xi and Gao [4] for more detail). Bollobas and Erdos [5] introduced the general Randic index, i.e.

$$R_\alpha(G) = \sum_{uv\in E(G)} (d(u)d(v))^\alpha,$$

where $d(u)$ denotes the degree of vertex u in molecular graph G. Li and Liu[6] determined the first three minimum general Randic indices among trees, and the corresponding extremal trees are characterized. Liu and Gutman [7] reported several novel estimates of the general Randic index and of its special cases – the ordinary and modified Zagreb indices.
Eliasi and Iranmanesh[8] defined the ordinary geometric-arithmetic index (or, general geometric-arithmetic index) as follows:

$$OGA_k(G) = \sum_{uv\in E(G)} \left[\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}\right]^k,$$

where k is a real number.

Let $e=uv$ be an edge of the molecular graph G. The number of edges of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $m_u(e)$. Analogously, $m_v(e)$ is the number of edges of G whose distance to the vertex v is smaller than the distance to the vertex u. Note that edges equidistant to u and v are not counted. Zhou et al., [9] proposed a third class of geometric-arithmetic index:

$$GA_3(G) = \sum_{e=uv\in E(G)} \frac{2\sqrt{m_u(e)m_v(e)}}{m_u(e)+m_v(e)}.$$

Let P_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 $\tilde{W}_n$.

In this paper, in terms of definitions and molecular graph structural analysis, we present the general Randic index of $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$. Also, the general geometric-arithmetic index and third geometric-arithmetic index of $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$ are derived. These results are new and illustrate the promising application prospects for biology and chemical sciences.

GENERAL RANDIC INDEX

Theorem 1. $R_\alpha(I_r(F_n)) = r(n+r)^k + 2((n+r)(2+r))^k + (n-2)((n+r)(3+r))^k$

$+ 2((2+r)(3+r))^k + (n-3)(3+r)^{2k} + 2r(2+r)^k + (n-2)r(3+r)^k$.

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 general Randic index, we have $R_\alpha(I_r(F_n))$

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

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

$+ (2((2+r)(3+r))^k + (n-3)((3+r)(3+r))^k) + (2r(2+r)^k + (n-2)r(3+r)^k)$. □

Corollary 1. $R_\alpha(F_n) = 2(2n)^k + (n-2)(3n)^k + 2\cdot 6^k + (n-3)\cdot 3^{2k}$.

Theorem 2. $R_\alpha(I_r(W_n)) = r(n+r)^k + n((n+r)(3+r))^k + n(3+r)^{2k} + nr(3+r)^k$.

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 general Randic index, we infer

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

$= r(n+r)^k + n((n+r)(3+r))^k + n((3+r)(3+r))^k + nr(3+r)^k$. □

corollary 2. $R_\alpha(W_n) = n(3n)^k + n\cdot 3^{2k}$.

Theorem 3. $R_\alpha(I_r(\tilde{F}_n)) = r(n+r)^k + 2((n+r)(2+r))^k + (n-2)((n+r)(3+r))^k + (n-2)r(3+r)^k +$

$2(2+r)^{2k} + 2(n-2)((3+r)(2+r))^k + (n+1)r(2+r)^k$.

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 general Randic index, we get

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

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

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

$(((2+r)(2+r))^k + (n-2)((3+r)(2+r))^k) + (((2+r)(2+r))^k + (n-2)((3+r)(2+r))^k) + (n-1)r(2+r)^k$. □

Corollary 3. $R_\alpha(\tilde{F}_n) = 2(2n)^k + (n-2)(3n)^k + 2\cdot 2^{2k} + 2(n-2)\cdot 6^k$.

Theorem 4. $R_\alpha(I_r(\tilde{W}_n)) = r(n+r)^k + n((n+r)(3+r))^k + nr(3+r)^k + 2n((3+r)(2+r))^k + nr(2+r)^k$.

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 $v_{i,i+1}$ ($1\le i\le n$). In view of the definition of general Randic index, we deduce

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

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

$$= r(n+r)^k + n((n+r)(3+r))^k + nr(3+r)^k + n((3+r)(2+r))^k + n((3+r)(2+r))^k + nr(2+r)^k.$$ □

Corollary 4. $R_\alpha(\tilde{W}_n) = n(3n)^k + 2n\cdot 6^k$.

GENERAL GEOMETRIC-ARITHMETIC INDEX

The terminologies for these special molecular graphs similar as Theorem 1- Theorem 4.

Theorem 5. $$OGA_k(I_r(F_n)) = r(\frac{2\sqrt{n+r}}{n+r+1})^k + 2(\frac{2\sqrt{(n+r)(2+r)}}{n+2r+2})^k + (n-2)(\frac{2\sqrt{(n+r)(3+r)}}{n+2r+3})^k$$

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

Proof. By the definition of general geometric-arithmetic index, we have

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

$$\sum_{i=1}^{n}\sum_{j=1}^{r}(\frac{2\sqrt{d(v_i)d(v_i^j)}}{d(v_i)+d(v_i^j)})^k$$

$$= r(\frac{2\sqrt{n+r}}{n+r+1})^k + (2(\frac{2\sqrt{(n+r)(2+r)}}{n+2r+2})^k + (n-2)(\frac{2\sqrt{(n+r)(3+r)}}{n+2r+3})^k)$$

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

Corollary 5. $$OGA_k(F_n) = 2(\frac{2\sqrt{2n}}{n+2})^k + (n-2)(\frac{2\sqrt{3n}}{n+3})^k + 2(\frac{2\sqrt{6}}{5})^k + (n-3).$$

Theorem 6. $$OGA_k(I_r(W_n)) = r(\frac{2\sqrt{n+r}}{n+r+1})^k + n(\frac{2\sqrt{(n+r)(3+r)}}{n+2r+3})^k + n + nr(\frac{2\sqrt{3+r}}{r+4})^k.$$

Proof. By the definition of general geometric-arithmetic index, we have

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

$$\sum_{i=1}^{n}\sum_{j=1}^{r}(\frac{2\sqrt{d(v_i)d(v_i^j)}}{d(v_i)+d(v_i^j)})^k$$

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

Corollary 6. $OGA_k(W_n) = n(\frac{2\sqrt{3n}}{n+3})^k + n$.

Theorem 7. $OGA_k(I_r(\tilde{F}_n)) = r(\frac{2\sqrt{n+r}}{n+r+1})^k + 2(\frac{2\sqrt{(n+r)(2+r)}}{n+2r+2})^k + (n-2)(\frac{2\sqrt{(n+r)(3+r)}}{n+2r+3})^k$

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

Proof. By virtue of the definition of general geometric-arithmetic index, we get

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

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

$$= r(\frac{2\sqrt{n+r}}{n+r+1})^k + (2(\frac{2\sqrt{(n+r)(2+r)}}{n+2r+2})^k + (n-2)(\frac{2\sqrt{(n+r)(3+r)}}{n+2r+3})^k)$$

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

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

Corollary 7. $OGA_k(\tilde{F}_n) = 2(\frac{2\sqrt{2n}}{n+2})^k + (n-2)(\frac{2\sqrt{3n}}{n+3})^k + 2+2(n-2)(\frac{2\sqrt{6}}{5})^k$.

Theorem 8. $OGA_k(I_r(\tilde{W}_n)) =$

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

Proof. In view of the definition of general geometric-arithmetic index, we deduce

$$OGA_k(I_r(\tilde{W}_n)) = \sum_{i=1}^{r}\left(\frac{2\sqrt{d(v)d(v^i)}}{d(v)+d(v^i)}\right)^k + \sum_{i=1}^{n}\left(\frac{2\sqrt{d(v)d(v_i)}}{d(v)+d(v_i)}\right)^k + \sum_{i=1}^{n}\sum_{j=1}^{r}\left(\frac{2\sqrt{d(v_i)d(v_i^j)}}{d(v_i)+d(v_i^j)}\right)^k +$$

$$\sum_{i=1}^{n}\left(\frac{2\sqrt{d(v_i)d(v_{i,i+1})}}{d(v_i)+d(v_{i,i+1})}\right)^k + \sum_{i=1}^{n}\left(\frac{2\sqrt{d(v_{i,i+1})d(v_{i+1})}}{d(v_{i,i+1})+d(v_{i+1})}\right)^k + \sum_{i=1}^{n}\sum_{j=1}^{r}\left(\frac{2\sqrt{d(v_{i,i+1})d(v_{i,i+1}^j)}}{d(v_{i,i+1})+d(v_{i,i+1}^j)}\right)^k$$

$$= r\left(\frac{2\sqrt{n+r}}{n+r+1}\right)^k + n\left(\frac{2\sqrt{(n+r)(3+r)}}{n+2r+3}\right)^k + nr\left(\frac{2\sqrt{3+r}}{r+4}\right)^k + n\left(\frac{2\sqrt{(3+r)(2+r)}}{2r+5}\right)^k + n\left(\frac{2\sqrt{(3+r)(2+r)}}{2r+5}\right)^k +$$

$$nr\left(\frac{2\sqrt{2+r}}{r+3}\right)^k . \square$$

Corollary 8. $OGA_k(\tilde{W}_n) = n\left(\frac{2\sqrt{3n}}{n+3}\right)^k + 2n\left(\frac{2\sqrt{6}}{5}\right)^k$.

THIRD GEOMETRIC-ARITHMETIC INDEX

Using the definition of third geometric-arithmetic index, we get the following computational formulas. The proving tricks are similar as Theorem 1- Theorem 4. We skip the detail proofs.

Theorem 9.

$$GA_3(I_r(F_n)) = \frac{4\sqrt{(2n+nr-r-4)(r+1)}}{2n+nr-3} + \frac{4\sqrt{(2n+nr-2r-4)(r+2)}}{2n+nr-r-2} +$$

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

$$+ \frac{2r(n+1)\sqrt{2n+r+nr-2}}{2n+r+nr-1}.$$

Corollary 9. $GA_3(F_n) = \frac{4\sqrt{2n-4}}{2n-3} + \frac{4\sqrt{n-2}}{n-1} + (n-4)\frac{2\sqrt{2(2n-5)}}{2n-3} + \sqrt{3} + \frac{4\sqrt{6}}{5} + (n-4)$.

Theorem 10. $GA_3(I_r(W_n)) = \frac{2n\sqrt{(r+2)(2n+nr-2r-5)}}{2n+nr-r-3} + n + \frac{2r(n+1)\sqrt{2n+r+nr-1}}{2n+r+nr}$.

Corollary 10. $GA_3(W_n) = \frac{2n\sqrt{2(2n-5)}}{2n-3} + n$.

Theorem 11. $GA_3(I_r(\tilde{F}_n)) = \frac{4\sqrt{(2r+1)(2nr+3n-2r-5)}}{2nr+3n-4} + \frac{(6n-8)\sqrt{(3r+2)(2nr+3n-3r-7)}}{2nr+3n-5}$

$$+\frac{4nr\sqrt{3n+2nr-3}}{3n+2nr-2}.$$

Corollary 11. $GA_3(\tilde{F}_n)=\frac{4\sqrt{3n-5}}{3n-4}+\frac{(6n-8)\sqrt{2(3n-7)}}{3n-5}$.

Theorem 12. $GA_3(I_r(\tilde{W}_n))=\frac{6n\sqrt{(3r+2)(2nr+3n-2r-5)}}{2nr+3n+r-3}+\frac{2r(2n+1)\sqrt{2nr+3n+r-1}}{2nr+3n+r}$.

Corollary 12. $GA_3(\tilde{W}_n)=\frac{6n\sqrt{2(3n-5)}}{3n-3}$.

CONCLUSION

In this paper, we determine the general Randic index, general geometric-arithmetic index and third geometric-arithmetic index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their *r*-corona molecular graphs. The general Randic index, general geometric-arithmetic index and third geometric-arithmetic index of more chemical structures should be considered in the future.

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