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Second Geometric-Arithmetic Index and General Sum Connectivity Index of Molecule Graphs with Special Structure

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Abstract

Second geometric-arithmetic index and general sum connectivity index as molecular graph invariant topological indices have been studied in recent years for prediction of chemical phenomena. In this paper, we determine the second geometric-arithmetic index and general sum connectivity index of molecular graph with special structures. At last, as supplemental results, we present the general geometric-arithmetic indices of certain molecular graphs.

Keywords: Molecule graph, second geometric-arithmetic index, general sum connectivity index

1. Introduction

Investigations of degree or distance based topological indices have been conducted over 35 years. Topological indices are numerical parameters of molecular graph which are invariant under graph isomorphisms. They play a significant role in physics, chemistry and pharmacology science.

Let G be the class of connected molecular graphs, then a topological index can be regarded as a score function f: $G \rightarrow \mathbb{R}^+$, with this property that $f(G_1) = f(G_2)$ if

G_1 and G_2 are isomorphic. As numerical descriptors of the molecular structure obtained from the corresponding molecular graph, topological indices have found several applications in theoretical chemistry, especially in QSPR/QSAR study. For instance, Wiener index, Hyper-Wiener index and edge average Wiener index are introduced to reflect certain structural features of organic molecules. Several papers contributed to determine these distance-based indices of special molecular graph (See Yan et al., [1] and [2], Gao and Shi [3], Gao and Wang [4], and Xi and Gao [5] for more detail).

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. We denote P_n and C_n are 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 [6] 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 $d(u)$ denotes the degree of vertex $u\in V(G)$. Several conclusions on GA index can refer to [7-9].

Recently, Fath-Tabar et al., [10] defined a new version of the geometric-arithmetic index, i.e., the second geometric-arithmetic index:

$$GA_2(G)=\sum_{uv\in E(G)}\frac{2\sqrt{n(u)n(v)}}{n(u)+n(v)},$$

where $n(u)$ is the number of vertices closer to vertex u than vertex v and $n(v)$ defines similarly. In Zhan and Qiao., [11], the maximum and the minimum second geometric-arithmetic index of the star-like tree are learned in view of an increasing or decreasing transformation of the second geometric arithmetic index of trees. Furthermore, they determine the corresponding extremal trees.

The sum connectivity index ($\chi(G)$) of molecular graph G are defined as:

$$\chi(G) = \sum_{uv\in E(G)} (d(u)+d(v))^{-\frac{1}{2}} .$$

Few years ago, Zhou and Trinajstic [12] introduced the general sum connectivity

$$\chi_k(G) = \sum_{uv\in E(G)} (d(u)+d(v))^{k} ,$$

where k is a real number. Some results on sum connectivity index and general sum connectivity index can refer to [13-23]

This paper is organized as follows. We first study the second geometric-arithmetic index for several molecular graphs with specific structure: r-crown molecular graph of fan molecular graph, wheel molecular graph, gear fan molecular graph and gear wheel molecular graph. Then, the general sum connectivity indices of these molecular graphs are determined.

2. Second Geometric-arithmetic Index

Theorem 1. $GA_2(I_r(F_n)) = \frac{4\sqrt{n-1}}{n} + 2(n-2)\frac{\sqrt{n-2}}{n-1} + \frac{4\sqrt{2}}{3} + (n-3) + 2r(n+1)\frac{\sqrt{r+n(r+1)}}{(n+1)(r+1)}$.

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. □

Using the definition of second geometric-arithmetic index, we have

$$GA_2(I_r(F_n)) = \sum_{i=1}^{r}\frac{2\sqrt{n(v)n(v^i)}}{n(v)+n(v^i)} + \sum_{i=1}^{n}\frac{2\sqrt{n(v)n(v_i)}}{n(v)+n(v_i)} + \sum_{i=1}^{n-1}\frac{2\sqrt{n(v_i)n(v_{i+1})}}{n(v_i)+n(v_{i+1})} + \sum_{i=1}^{n}\sum_{j=1}^{r}\frac{2\sqrt{n(v_i)n(v_i^j)}}{n(v_i)+n(v_i^j)}$$

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

Corollary 1. $GA_2(F_n) = \frac{4\sqrt{n-1}}{n} + 2(n-2)\frac{\sqrt{n-2}}{n-1} + \frac{4\sqrt{2}}{3} + (n-3)$.

Theorem 2. $GA_2(I_r(W_n)) = 2n\frac{\sqrt{n-2}}{n-1} + n + 2r(n+1)\frac{\sqrt{r+n(r+1)}}{(n+1)(r+1)}$.

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

In view of the definition of second geometric-arithmetic index, we infer

$$GA_2(I_r(W_n)) = \sum_{i=1}^{r}\frac{2\sqrt{n(v)n(v^i)}}{n(v)+n(v^i)} + \sum_{i=1}^{n}\frac{2\sqrt{n(v)n(v_i)}}{n(v)+n(v_i)} + \sum_{i=1}^{n}\frac{2\sqrt{n(v_i)n(v_{i+1})}}{n(v_i)+n(v_{i+1})} + \sum_{i=1}^{n}\sum_{j=1}^{r}\frac{2\sqrt{n(v_i)n(v_i^j)}}{n(v_i)+n(v_i^j)}$$

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

Corollary 2. $GA_2(W_n) = 2n\frac{\sqrt{n-2}}{n-1} + n$.

Theorem 3. $GA_2(I_r(\tilde{F}_n)) = 4\frac{\sqrt{n-1}}{n} + 2r\frac{\sqrt{2n(r+1)-1}}{r+1} + (3n-4)\frac{\sqrt{3(2n-3)}}{n}$.

Proof. Let $P_n=v_1v_2\dots v_n$ 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 $v_{i,i+1}$ $(1 \le i \le n\text{-}1)$. 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 second geometric-arithmetic index, we yield

$$GA_2(I_r(\tilde{F}_n)) = \sum_{i=1}^{r}\frac{2\sqrt{n(v)n(v^i)}}{n(v)+n(v^i)} + \sum_{i=1}^{n}\frac{2\sqrt{n(v)n(v_i)}}{n(v)+n(v_i)} + \sum_{i=1}^{n}\sum_{j=1}^{r}\frac{2\sqrt{n(v_i)n(v_i^j)}}{n(v_i)+n(v_i^j)} +$$

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

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

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

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

Corollary 3. $GA_2(\tilde{F}_n)=4\frac{\sqrt{n-1}}{n}+(3n-4)\frac{\sqrt{3(2n-3)}}{n}$.

Theorem 4. $GA_2(I_r(\tilde{W}_n))=6n\frac{\sqrt{3(2n-2)}}{2n+1}+2r(2n+1)\frac{\sqrt{r+2n(r+1)}}{(2n+1)(r+1)}$.

Proof. Let $C_n=v_1v_2\dots v_n$ and v be a vertex in W_n beside C_n, and $v_{i,i+1}$ 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 second geometric-arithmetic index, we deduce

$$GA_2(I_r(\tilde{W}_n)) = \sum_{i=1}^{r}\frac{2\sqrt{n(v)n(v^i)}}{n(v)+n(v^i)} + \sum_{i=1}^{n}\frac{2\sqrt{n(v)n(v_i)}}{n(v)+n(v_i)} + \sum_{i=1}^{n}\sum_{j=1}^{r}\frac{2\sqrt{n(v_i)n(v_i^j)}}{n(v_i)+n(v_i^j)} + \sum_{i=1}^{n-1}\frac{2\sqrt{n(v_i)n(v_{i,i+1})}}{n(v_i)+n(v_{i,i+1})}$$

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

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

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

Corollary 4. $GA_2(\tilde{W}_n)=6n\frac{\sqrt{3(2n-2)}}{2n+1}$.

3. General Sum Connectivity Index

Theorem 5. $\chi_k(I_r(F_n)) = r(n+r+1)^k + 2(n+2r+2)^k+(n-2)(n+2r+3)^k + 2(2r+5)^k+(n-3)(2r+6)^k+2r(r+3)^k+(n-2)r(r+4)^k$.

Corollary 5. $\chi_k(F_n)=2(n+2)^k+(n-2)(n+3)^k+2\cdot 5^k+(n-3)\cdot 6^k$.

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

Corollary 7. $\chi(F_n)=\frac{2}{\sqrt{n+2}}+\frac{n-2}{\sqrt{n+3}}+\frac{2}{\sqrt{5}}+\frac{n-3}{\sqrt{6}}$.

Theorem 6. $\chi_k(I_r(W_n))=r(n+r+1)^k+n(n+2r+3)^k+n(2r+6)^k+nr(r+4)^k$.

Corollary 8. $\chi_k(W_n) = n(n+3)^k + n \cdot 6^k$.

Corollary 9. $\chi(I_r(W_n)) = \frac{r}{\sqrt{n+r+1}} + \frac{n}{\sqrt{n+2r+3}} + \frac{n}{\sqrt{2r+6}} + \frac{nr}{\sqrt{r+4}}$.

Corollary 10. $\chi(W_n) = \frac{n}{\sqrt{n+3}} + \frac{n}{\sqrt{6}}$.

Theorem 7. $\chi_k(I_r(\tilde{F}_n)) = r(n+r+1)^k + 2(n+2r+2)^k + (n-2)(n+2r+3)^k +$ $(n-2)r(r+4)^k + 2(2r+4)^k + 2(n-2)(2r+5)^k + (n+1)r(r+3)^k$.

Corollary 11. $\chi_k(\tilde{F}_n) = 2(n+2)^k + (n-2)(n+3)^k + 2 \cdot 4^k + 2(n-2) \cdot 5^k$.

Corollary12. $\chi(I_r(\tilde{F}_n)) = \frac{r}{\sqrt{n+r+1}} + \frac{2}{\sqrt{n+2r+2}} + \frac{n-2}{\sqrt{n+2r+3}} + \frac{(n-2)r}{\sqrt{r+4}} +$ $\frac{2}{\sqrt{2r+4}} + \frac{2(n-2)}{\sqrt{2r+5}} + \frac{(n+1)r}{\sqrt{r+3}}$.

Corollary 13. $\chi(\tilde{F}_n) = \frac{2}{\sqrt{n+2}} + \frac{n-2}{\sqrt{n+3}} + 1 + \frac{2(n-2)}{\sqrt{5}}$.

Theorem 8. $\chi_k(I_r(\tilde{W}_n)) = r(n+r+1)^k + n(n+2r+3)^k + nr(r+4)^k + 2n(2r+5)^k +$ $nr(r+3)^k$.

Corollary 14. $\chi_k(\tilde{W}_n) = n(n+3)^k + 2n \cdot 5^k$.

Corollary 15. $\chi(I_r(\tilde{W}_n)) = \frac{r}{\sqrt{n+r+1}} + \frac{n}{\sqrt{n+2r+3}} + \frac{nr}{\sqrt{r+4}} + \frac{2n}{\sqrt{2r+5}} + \frac{nr}{\sqrt{r+3}}$.

Corollary 16. $\chi(\tilde{W}_n) = \frac{n}{\sqrt{n+3}} + \frac{2n}{\sqrt{5}}$.

4. Extension Results

At last of our paper, we present some conclusions on general geometric-arithmetic index ($OGA_k(G)=\sum_{uv\in E(G)}[\frac{2\sqrt{d(u)d(v)}}{d(u)+d(v)}]^k$ where k is a real number) as supplemental results. We skip the detail proofs.

Theorem 9. Let K_n be the complete molecular graph with n vertices. Then, $OGA_k(K_n)=\frac{n(n-1)}{2}$.

Theorem 10. Let G be a regular molecular graph with degree r>0 and order n. Then $OGA_k(G)=\frac{nr}{2}$.

Theorem 11. Let S_n be a star molecular graph with n+1 vertices. Then

$OGA_k(S_n)=n(\frac{2\sqrt{n}}{n+1})^k$.

Let $NS_1[n]$ and $NS_2[n]$ be two infinite classes of nanostar dendrimers presented in Madanshekaf and Moradi [9].

Theorem 12.

$$OGA_k(NS_1[n])=2^{n+1}(\frac{2\sqrt{2}}{3})^k+(3\cdot 2^{n+2}-11)+(2^{n+2}-4)(\frac{\sqrt{3}}{2})^k+(7\cdot 2^{n+1}-4)(\frac{2\sqrt{6}}{5})^k,$$

$$OGA_k(NS_2[n])=2^{n+1}(\frac{2\sqrt{2}}{3})^k+(2^{n+3}-5)+(3\cdot 2^{n+1}-6)(\frac{2\sqrt{6}}{5})^k.$$

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