The General Sum-Connectivity Co-Index and General Second Zagreb Co–Index of Certain Crown Molecular Graphs

Yun Gao
Department of Editorial, Yunnan Normal University, Kunming 650092, China
gy64gy@sina.com

Wei Gao, Li Liang,
School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China

***Abstract*: As molecular graph invariant topological indices, the first and second Zagreb co–index, general sum-connectivity co-index and general second Zagreb co–index have been studied in recent years for prediction of chemical phenomena. In this paper, in terms of strict mathematical deduction, we determine the general sum-connectivity co-index and general second Zagreb co–index of certain *r*-crown molecular graphs.**

Keywords: Molecule graph, general sum-connectivity co-index, general second Zagreb co–index, r-crown molecular graph

I.INTRODUCTION

In recent years, as a branch of theoretical chemistry, chemical graph theory caused widespread concern of scholars. Let *G* be the class of connected molecular graphs, then a topological index can be regarded as a score function *f*: $G \to \mathbb{R}^+$, 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, Hyener 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], Gao et al., [2], Gao and Shi [3], Gao and Wang [4], and Xi and Gao [5, 6] for more detail).

The molecular graphs considered in our paper are all simple. 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 $\widetilde{F}_n$. 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 $\widetilde{W}_n$

For a molecular graph *G*, the first Zagreb co–index of *G* is defined as [7]:

$$\bar{M}_1(G) = \sum_{uv \notin E(G)} (d(u)+d(v)),$$

where $d(u)$ denotes the degree of vertex *v* in molecular graph *G*. Su and Xu [8] introduced a new invariant, the general sum-connectivity co-index, which is defined as

$$\bar{\chi}_\alpha(G) = \sum_{uv \notin E(G)} (d(u)+d(v))^\alpha,$$

where α is a real number.

The second Zagreb co–index of molecular graph G is defined by Babujee and Ramakrishnan [9]:

$$\bar{M}_2(G) = \sum_{uv \notin E(G)} (d(u)d(v)).$$

Inspired by general sum-connectivity co-index, we expend the second Zagreb co–index and define its general version. Let α be a real number, then the general second Zagreb co–index of molecular graph *G* is denoted as

$$\bar{M}_2^{\alpha}(G)=\sum_{uv\notin E(G)}(d(u)d(v))^{\alpha}.$$

Although there have been several advances in general sum-connectivity co-index and general second Zagreb co–index of molecular graphs, the study of general sum-connectivity co-index and general second Zagreb co–index of special chemical structures has been largely limited. In addition, as widespread and critical chemical structures, *r*-crown molecular graph are widely used in medical science and pharmaceutical field. For these reasons, we have attracted tremendous academic and industrial interests to research the general sum-connectivity co-index and general second Zagreb co–index of special *r*-crown molecular structures from a mathematical point of view.

The contributions of our paper are two-fold. We first study the general sum-connectivity co-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 second Zagreb co–index of these molecular graphs are determined.

II GENERAL SUM-CONNECTIVITY CO-INDEX

Theorem1. $\bar{\chi}_{\alpha}(I_r(F_n)) = nr(n+r+1)^{\alpha} + (2n-6)(2r+5)^{\alpha}+\frac{(n-4)(n-3)}{2}(2r+6)^{\alpha}+(2r+4)^{\alpha}+2rn(r+3)^{\alpha}+rn(n-2)(r+4)^{\alpha}+\frac{r^2n^2-rn}{2}2^{\alpha}$.

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.

In view of the definition of general sum-connectivity co-index, we deduce

$$\bar{\chi}_{\alpha}(I_r(F_n))=\sum_{i=1}^{r}\sum_{j=1}^{n}(d(v^i)+d(v_j))^{\alpha}$$

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

$$+\sum_{i,j\in\{1,\cdots,n\},|i-j|\ge 2}(d(v_i)+d(v_j))^{\alpha}+\sum_{i\ne j}\sum_{k=1}^{r}(d(v_i)+d(v_j^k))^{\alpha}$$

$$+\sum_{i=1}^{n}\sum_{j,k\in\{1,\cdots,r\},j\ne k}(d(v_i^j)+d(v_i^k))^{\alpha}+\sum_{i,j\in\{1,\cdots,n\},i\ne j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)+d(v_j^t))^{\alpha}$$

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

Corollary1. $\bar{\chi}_{\alpha}(F_n)=(2n-6)\cdot 5^{\alpha}+\frac{(n-4)(n-3)}{2}\cdot 6^{\alpha}+4^{\alpha}$.

Corollary2. $\bar{M}_1(I_r(F_n)) = r^2(2n^2+n)+r(6n^2-5n+2)+(3n^2-11n+10)$.

Corollary 3. $\bar{M}_1(F_n)=3n^2-11n+10$.

Theorem2. $\bar{\chi}_{\alpha}(I_r(W_n))=nr(n+r+1)^{\alpha}+\frac{n(n-3)}{2}(2r+6)^{\alpha}+rn^2(r+4)^{\alpha}+\frac{r^2n^2+2nr^2-nr}{2}2^{\alpha}$.

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*. We denote $v_nv_{n+1}=v_nv_1$.

In terms of the definition of general sum-connectivity co-index, we infer

$$\overline{\chi}_\alpha(I_r(W_n))=\sum_{i=1}^{r}\sum_{j=1}^{n}(d(v^i)+d(v_j))^\alpha$$

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

$$+\sum_{i,j\in\{1,\cdots,n\},|i-j|\geq 2,(i,j)\neq(1,n)}(d(v_i)+d(v_j))^\alpha+$$

$$\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}(d(v_i)+d(v_j^k))^\alpha$$

$$+\sum_{i=1}^{n}\sum_{j,k\in\{1,\cdots,r\},j\neq k}(d(v_i^j)+d(v_i^k))^\alpha$$

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)+d(v_j^t))^\alpha$$

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

$$+rn(n-1)(r+4)^\alpha+\frac{nr(r-1)}{2}2^\alpha+\frac{r^2n(n-1)}{2}2^\alpha$$

Corollary4. $\overline{\chi}_\alpha(W_n)=\frac{n(n-3)}{2}\cdot 6^\alpha$.

Corollary5. $\overline{M}_1(I_r(W_n))= r^2(2n^2+3n)+r(6n^2-3n)$ $+(3n^2-9n)$.

Corollary6. $\overline{M}_1(W_n)=3n^2-9n$.

Theorem3. $\overline{\chi}_\alpha(I_r(\tilde{F}_n))=(n^2-3n+2)(2r+5)^\alpha$

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

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

$$+(n^2+2n-1)r(r+3)^\alpha+(2n-1)r(n+r+1)^\alpha$$

$$+(n-2)(2n-1)r(4+r)^\alpha.$$

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, $v_i^2,\dots,$ v_i^r be the r hanging vertices of v_i ($1\leq i\leq n$). Let $v_{i,i+1}^1$, $v_{i,i+1}^2,\dots,$ $v_{i,i+1}^r$ 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.

Using the definition of general sum-connectivity co-index, we obtain

$$\overline{\chi}_\alpha(I_r(\tilde{F}_n))=\{\sum_{i=1}^{r}\sum_{j=1}^{n}(d(v^i)+d(v_j))^\alpha$$

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

$$+\sum_{i,j\in\{1,\cdots,n\}}(d(v_i)+d(v_j))^\alpha\sum_{i\neq j}\sum_{k=1}^{r}(d(v_i)+d(v_j^k))^\alpha$$

$$+\sum_{i=1}^{n}\sum_{j,k\in\{1,\cdots,r\},j\neq k}(d(v_i^j)+d(v_i^k))^\alpha$$

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)+d(v_j^t))^\alpha\}+$$

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

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

$$+\sum_{i,j\in\{1,\cdots,n-1\},i\neq j}(d(v_{i,i+1})+d(v_{j,j+1}))^\alpha$$

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

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

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

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

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

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

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

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

$\frac{r^2n(n-1)}{2}2^{\alpha}\ \}+\{\ (n-1)r(r+3)^{\alpha}\ +(n-1)(n+2r+2)^{\alpha}$

$+((2n-4)(2r+4)^{\alpha}+(n-2)(n-3)(2r+6)^{\alpha})$

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

$+(n-1)r^2\cdot 2^{\alpha}+(n-1)r(n+r+1)^{\alpha}$

$+(2(n-1)r(3+r)^{\alpha}+(n-2)(n-1)r(4+r)^{\alpha})$

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

Corollary7. $\overline{\chi}_{\alpha}(\tilde{F}_n)=(n^2-3n+2)\cdot 5^{\alpha}+(n-1)(n+2)^{\alpha}+\frac{(n-2)(n-3)}{2}\cdot 6^{\alpha}+(\frac{n^2}{2}+\frac{n}{2}-2)\cdot 4^{\alpha}.$

Corollar8. $\overline{M}_1(I_r(\tilde{F}_n))=r^2(5n^2+n-1)+r(17n^2-23n+9)+(11n^2-27n+18).$

Corollary9. $\overline{M}_1(\tilde{F}_n)=11n^2-27n+18.$

Theorem4. $\overline{\chi}_{\alpha}(I_r(\tilde{W}_n))=2nr(n+r+1)^{\alpha}+(\frac{1}{2}n^2-\frac{1}{2}n)(2r+6)^{\alpha}\ +\ rn(2n-1)(r+4)^{\alpha}\ +\ (n^2-2n)(2r+5)^{\alpha}\ +(r^2n^2+2nr^2-nr)2^{\alpha}+n(n+2r+2)^{\alpha}+\frac{n(n-1)}{2}(2r+4)^{\alpha}+n^2r(r+3)^{\alpha}.$

Proof. Let $C_n=v_1v_2\ldots v_n$ 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 $v_{n.n+1}=v_{n.1}$, $v_{n+1}=v_1$.

By virtue of the definition of general sum-connectivity co-index, we get

$$\overline{\chi}_{\alpha}(I_r(\tilde{W}_n))=\{\sum_{i=1}^{r}\sum_{j=1}^{n}(d(v^i)+d(v_j))^{\alpha}+$$

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

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}(d(v_i)+d(v_j))^{\alpha}$$

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}(d(v_i)+d(v_j^k))^{\alpha}$$

$$+\sum_{i=1}^{n}\sum_{j,k\in\{1,\cdots,r\},j\neq k}(d(v_i^j)+d(v_i^k))^{\alpha}$$

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)+d(v_j^t))^{\alpha}\ \}$$

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

$$+\sum_{i=1}^{n}\sum_{j\notin\{i,i+1\}}(d(v_{i,i+1})+d(v_j))^{\alpha}$$

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}(d(v_{i,i+1})+d(v_{j,j+1}))^{\alpha}$$

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

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

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

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

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

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_{i,i+1}^{k})+d(v_{j,j+1}^{t}))^{\alpha}\}$$

$$=\{nr(r+4)^{\alpha}+nr^{2}2^{\alpha}+nr(n+r+1)^{\alpha}+\frac{n(n-1)}{2}(2r+6)^{\alpha}+$$

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

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

$$+(n-1)nr(r+3)^{\alpha}+nr^{2}\cdot 2^{\alpha}+nr(n+r+1)^{\alpha}$$

$$+n(n-1)r(4+r)^{\alpha}+\frac{nr(r-1)}{2}2^{\alpha}+\frac{(n-1)n}{2}r^{2}2^{\alpha}\}.$$

Corollary10. $\bar{\chi}_{\alpha}(\tilde{W}_{n})=(\frac{1}{2}n^{2}-\frac{1}{2}n)\cdot 6^{\alpha}+(n^{2}-2n)\cdot 5^{\alpha}+n(n+2)^{\alpha}+\frac{n(n-1)}{2}\cdot 4^{\alpha}$

Corollary11. $\bar{M}_{1}(I_{r}(\tilde{W}_{n}))=2nr(n+r+1)+(\frac{1}{2}n^{2}-\frac{1}{2}n)(2r+6)+rn(2n-1)(r+4)+(n^{2}-2n)(2r+5)+(r^{2}n^{2}+2nr^{2}-nr)2+n(n+2r+2)+\frac{n(n-1)}{2}(2r+4)+n^{2}r(r+3)$.

$$=r^{2}(5n^{2}+5n)+r(17n^{2}-8n)+(11n^{2}-13n).$$

Corollary12. $\bar{M}_{1}(\tilde{W}_{n})=11n^{2}-13n$.

III.GENERAL SECOND ZAGREB CO-INDEX

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

Theorem5. $\bar{M}_{2}^{\alpha}(I_{r}(F_{n}))=(2nr+1)(r+2)^{\alpha}+nr(n+r)^{\alpha}+(2n-6)((r+2)(r+3))^{\alpha}+\frac{(n-4)(n-3)}{2}(r+3)^{2\alpha}+r(n-2)n(r+3)^{\alpha}+\frac{r^{2}n^{2}+2nr^{2}-nr}{2}$.

Proof. Using the definition of general second Zagreb co–index, we have

$$\bar{M}_{2}^{\alpha}(I_{r}(F_{n}))=\sum_{i=1}^{r}\sum_{j=1}^{n}(d(v^{i})d(v_{j}))^{\alpha}$$

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

$$+\sum_{i,j\in\{1,\cdots,n\},|i-j|\geq 2}(d(v_{i})d(v_{j}))^{\alpha}+\sum_{i\neq j}\sum_{k=1}^{r}(d(v_{i})d(v_{j}^{k}))^{\alpha}$$

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

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_{i}^{k})d(v_{j}^{t}))^{\alpha}$$

$$=(2r(r+2)^{\alpha}+(n-2)r(r+3)^{\alpha})+nr^{2}+nr(n+r)^{\alpha}+$$

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

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

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

Corollary13. $\bar{M}_{2}^{\alpha}(F_{n})=2^{\alpha}+(2n-6)\cdot 6^{\alpha}+\frac{(n-4)(n-3)}{2}\cdot 3^{2\alpha}$.

Corollary14. $\bar{M}_{2}(I_{r}(F_{n}))=r^{2}(2n^{2}+\frac{1}{2}n)+r(7n^{2}-\frac{27}{2}n+7)+(\frac{9}{2}n^{2}-\frac{39}{2}n+20)$.

Corollary15. $\bar{M}_{2}(F_{n})=\frac{9}{2}n^{2}-\frac{39}{2}n+20$.

Theorem6. $\bar{M}_{2}^{\alpha}(I_{r}(W_{n}))=nr(n+r)^{\alpha}+\frac{n(n-3)}{2}(r+3)^{2\alpha}+rn^{2}(r+3)^{\alpha}+\frac{r^{2}n^{2}+2nr^{2}-nr}{2}$.

Proof. In view of the definition of general second Zagreb co–index, we infer

$$\bar{M}_{2}^{\alpha}(I_{r}(W_{n}))=\sum_{i=1}^{r}\sum_{j=1}^{n}(d(v^{i})d(v_{j}))^{\alpha}$$

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

$$+\sum_{i,j\in\{1,\cdots,n\},|i-j|\geq 2,(i,j)\neq(1,n)}(d(v_i)d(v_j))^{\alpha}$$

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}(d(v_i)d(v_j^k))^{\alpha}$$

$$+\sum_{i=1}^{n}\sum_{j,k\in\{1,\cdots,r\},j\neq k}(d(v_i^j)d(v_i^k))^{\alpha}$$

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)d(v_j^t))^{\alpha}$$

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

$$rn(n-1)(r+3)^{\alpha}+\frac{nr(r-1)}{2}+\frac{r^2n(n-1)}{2}.$$

Corollary16. $\bar{M}_2^{\alpha}(W_n)=\frac{n(n-3)}{2}3^{2\alpha}$.

Corollary17. $\bar{M}_2(I_r(W_n))= r^2(2n^2+\frac{n}{2})+r(7n^2-\frac{19}{2}n)$

$$+(\frac{9}{2}n^2-\frac{27}{2}n).$$

Corollary18. $\bar{M}_2(W_n)=\frac{9}{2}n^2-\frac{27}{2}n$.

Theorem7. $\bar{M}_2^{\alpha}(I_r(\tilde{F}_n))=\frac{(n-2)(n-3)}{2}(r+3)^{2\alpha}+$

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

$$+(n-2)(n-1)((r+2)(r+3))^{\alpha}+(\frac{n^2}{2}+\frac{n}{2}-2)(r+2)^{2\alpha}$$

$$+(n+3)(n-1)r(r+2)^{\alpha}+(2n-1)r(n+r)^{\alpha}$$

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

Proof. By virtue of the definition of general second Zagreb co–index, we yield

$$\bar{M}_2^{\alpha}(I_r(\tilde{F}_n))=\{\sum_{i=1}^{r}\sum_{j=1}^{n}(d(v^i)d(v_j))^{\alpha}+\sum_{i=1}^{r}\sum_{j=1}^{n}\sum_{k=1}^{r}(d(v^i)d(v_j^k))^{\alpha}+$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}(d(v)d(v_i^j))^{\alpha}+\sum_{i,j\in\{1,\cdots,n\}}(d(v_i)d(v_j))^{\alpha}+$$

$$\sum_{i\neq j}\sum_{k=1}^{r}(d(v_i)d(v_j^k))^{\alpha}+\sum_{i=1}^{n}\sum_{j,k\in\{1,\cdots,r\},j\neq k}(d(v_i^j)d(v_i^k))^{\alpha}$$

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)d(v_j^t))^{\alpha}\}+$$

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

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

$$+\sum_{i,j\in\{1,\cdots,n-1\},i\neq j}(d(v_{i,i+1})d(v_{j,j+1}))^{\alpha}$$

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

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

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

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

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

$$=\{(2r(r+2)^{\alpha}+(n-2)r(r+3)^{\alpha})+nr^2+nr(n+r)^{\alpha}$$

$$+((r+2)^{2\alpha}+(2n-4)((r+2)(r+3))^{\alpha}$$

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

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

$$\{(n-1)r(r+2)^{\alpha}+(n-1)((n+r)(r+2))^{\alpha}+((2n-4)(r+2)^{2\alpha}$$

$$+(n-2)(n-3)((r+2)(r+3))^{\alpha})+\frac{(n-1)(n-2)}{2}(r+2)^{2\alpha}$$

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

$$+(2(n-1)r(2+r)^{\alpha}+(n-2)(n-1)r(3+r)^{\alpha})$$

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

Corollary19. $\bar{M}_2^{\alpha}(\tilde{F}_n)=\frac{(n-2)(n-3)}{2}3^{2\alpha}+(n-1)(2n)^{\alpha}$

$+(n-2)(n-1)\cdot 6^{\alpha}+(\frac{n^2}{2}+\frac{n}{2}-2)\cdot 2^{2\alpha}$.

Corollary20. $\bar{M}_2(I_r(\tilde{F}_n))=r^2(\frac{9}{2}n^2-9n+\frac{11}{2})$

$+r(22n^2-36n+\frac{29}{2})+(\frac{29}{2}n^2-\frac{81}{2}n+31)$.

Corollary21. $\bar{M}_2(\tilde{F}_n)=\frac{29}{2}n^2-\frac{81}{2}n+31$.

Theorem8. $\bar{M}_2^{\alpha}(I_r(\tilde{W}_n))=nr(n+r)^{\alpha}+(\frac{3}{2}n^2-\frac{5}{2}n)(r+3)^{2\alpha}+n^2r^2+2nr^2-nr+n((n+r)(r+2))^{\alpha}+\frac{n(n-1)}{2}(r+2)^{2\alpha}+n^2r(r+2)^{\alpha}+nr(n+r)^{\alpha}+n(2n-1)r(3+r)^{\alpha}$.

Proof. In view of the definition of general second Zagreb co–index, we deduce

$$\bar{M}_2^{\alpha}(I_r(\tilde{W}_n))=\{\sum_{i=1}^{r}\sum_{j=1}^{n}(d(v^i)d(v_j))^{\alpha}$$

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

$$\sum_{i,j\in\{1,\cdots,n\},i\neq j}(d(v_i)d(v_j))^{\alpha}+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}(d(v_i)d(v_j^k))^{\alpha}$$

$$+\sum_{i=1}^{n}\sum_{j,k\in\{1,\cdots,r\},j\neq k}(d(v_i^j)d(v_i^k))^{\alpha}+$$

$$\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_i^k)d(v_j^t))^{\alpha}\}$$

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

$$+\sum_{i=1}^{n}\sum_{j\notin\{i,i+1\}}(d(v_{i,i+1})d(v_j))^{\alpha}+\sum_{i,j\in\{1,\cdots,n\},i\neq j}(d(v_{i,i+1})d(v_{j,j+1}))^{\alpha}$$

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

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

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

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

$$+\sum_{i,j\in\{1,\cdots,n\},i\neq j}\sum_{k=1}^{r}\sum_{t=1}^{r}(d(v_{i,i+1}^k)d(v_{j,j+1}^t))^{\alpha}\}$$

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

Corollary22. $\bar{M}_2^{\alpha}(\tilde{W}_n)=(\frac{3}{2}n^2-\frac{5}{2}n)\cdot 3^{2\alpha}+n(2n)^{\alpha}+\frac{n(n-1)}{2}\cdot 2^{2\alpha}$.

Corollary23. $\bar{M}_2(I_r(\tilde{W}_n))=r^2(6n^2+n)+r(22n^2-19n)+(\frac{35}{2}n^2-\frac{49}{2}n)$.

Corollary24. $\bar{M}_2(\tilde{W}_n)=\frac{35}{2}n^2-\frac{49}{2}n$.

IV.CONCLUSION

In this paper, by virtue of definitions and molecular graph structural analysis, we determine the general sum-connectivity co-index and general second Zagreb co–index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their *r*-corona molecular graphs. The general sum-connectivity co-index and general second Zagreb co–index of more chemical structures should be considered in the future.

V.ACKNOWLEDGEMENTS

First, we thank the reviewers for their constructive comments in improving the quality of this paper. This work was supported in part by NSFC (no. 11401519). We also would like to thank the anonymous referees for providing us with constructive comments and suggestions.

REFERENCES

[1] L. Yan, Y. Li, W. Gao, J. Li, On the extremal hyper-wiener index of graphs, Journal of Chemical and Pharmaceutical Research, 2014, 6(3): 477-481.

[2] W. Gao, L. Liang, Y. Gao, Some results on wiener related index and shultz index of molecular graphs, Energy Education Science and Technology: Part A, 2014, 32(6): 8961-8970.

[3] W. Gao, L. Shi, Wiener index of gear fan graph

co–indices of graph operations, Discrete Applied Mathematics, 2010, 158: 1571- 1578.

[8] G. F. Su, L. Xu, On the general sum–connectivity co–index of graphs, Iranian Journal of

and gear wheel graph, Asian Journal of Chemistry, 2014, 26(11): 3397-3400.

[4] W. Gao, W. F. Wang, Second atom-bond connectivity index of special chemical molecular structures, Journal of Chemistry, Volume 2014,Article ID906254,8pages, http://dx.doi.org/10.1155/2014/906254.

[5] W. F. Xi, W. Gao, Geometric-arithmetic index and Zagreb indices of certain special molecular graphs, Journal of Advances in Chemistry, 2014, 10(2): 2254-2261.

[6] W. F. Xi, W. Gao, λ -Modified extremal hyper-Wiener index of molecular graphs, Journal of Applied Computer Science & Mathematics, 2014, 18 (8): 43-46.

[7] A. R. Ashrafi, T. Doslic, A. Hamzeh, The Zagreb

Mathematical Chemistry, 2011, 2(1): 89-98.

[9] J. B. Babujee, S. Ramakrishnan, Topological indices and new graph structures, Applied Mathematical Sciences, 2012, 6(108): 5383-5401.