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Three Indices Calculation of Certain Crown Molecular Graphs

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Abstract: As molecular graph invariant topological indices, harmonic index, zeroth-order general Randic index and Co-PI index have been studied in recent years for prediction of chemicalphenomena. In this paper, we determine the harmonic index, zeroth-order general Randic index andCo-PI indexof certain r-crown molecular graphs.

Keywords: Molecule graph; harmonic index; zeroth-order general Randic index; Co-PI index; r-crown molecular graph

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1. INTRODUCTION

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 fromthe corresponding molecular graph, topological indices have found several applications in theoretical chemistry, especially in QSPR/QSAR study. For instance, Wiener index,Hyper-Wiener indexand 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] 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 $\tilde{F}_n$. 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 $\tilde{W}_n$.

For a molecular graph G, the harmonic index is defined as:

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

where $d(v)$ denotes as the degree of vertex v in molecular graph G.

Favaronet al.,[6] presented the relation between harmonic index and the eigenvalues of molecular graphs. Zhong [7] determined the minimum and maximum values of the harmonic index for connected molecular graphs and trees, and characterized the corresponding extremalmolecular graphs. Recently, Wu et al.,[8] obtained the minimum value of the harmonic index among the molecular graphs with the minimum degree at least two. Liu [9] gave several relations between the harmonic index and diameter of molecular graphs.

The zeroth-order general Randic indexof molecular graph G is defined as

$$\chi_\alpha(G)=\sum_{v\in V(G)} d(v)^\alpha,$$

where α is a real number.

For $\alpha > 1$or $\alpha < 0$, Zhang and Zhou [10] characterized respectively the n-vertex trees and the n-vertex unicyclicmolecular graphs of fixed number of pendent vertices with the first three largest zeroth-ordergeneral Randic indices, and they also discussed respectively the n-vertex trees andthe n-vertex unicyclicmolecular graphs of fixed maximum degree with the first two largestzeroth-order general Randic indices.Pavlovic [11] yielded the zeroth-order general Randic indexof connected graph without loops and multiple edges.

Let $e=uv$ be an edge of the molecular graph G. The number of vertices of G whose distance to the vertex u is smaller than thedistance to the vertex v is denoted by $n_u(e)$. Analogously, $n_v(e)$ is the number of vertices of$G$ whose distance to the vertex$v$ is smaller than the distance to the vertex u. Note that vertices equidistant to u and v are not counted. Hasani et al., [12] introduced Co-PI index as

$$Co-PI_v(G)=\sum_{e=uv\in E(G)}|n_u(e)-n_u(e)|.$$

Su et al., [13] proved that $Co-PI_v(G)=\sum_{e=uv\in E(G)}|T(u)-T(v)|$, where $T(u)=T_G(u)=\sum_{v\in V}d_G(u,v)$.

The contributions of our paper are three-fold.We first study the harmonic indexfor several molecular graphs with specific structure: r- crown molecular graph of fan molecular graph, wheel molecular graph, gear fan molecular graph andgear wheel molecular graph.Then, the zeroth-order general Randic indexes of these molecular graphs are determined. At last, we present the Co-PI indexof these molecular graphs.

1. HARMONIC INDEX

Theorem 1. $H(I_r(F_n))=\frac{2r}{n+r+1}+\frac{4}{n+2r+2}+\frac{2(n-2)}{n+2r+3}+\frac{4}{2r+5}+\frac{n+4r-3}{r+3}+\frac{2(n-2)r}{r+4}$.

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.□

In view of the definition of harmonic index, we deduce

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

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

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

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

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

In terms of the definition ofharmonic index, we infer

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

$= \frac{2r}{n+r+1} + \frac{2n}{n+2r+3} + \frac{2n}{2r+6} + \frac{2nr}{r+4}$. □

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

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

Proof. Let $P_n = v_1 v_2 \ldots v_n$ 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.

Using the definition ofharmonic index, we obtain

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

$$= \frac{2r}{n+r+1} + \left(\frac{4}{n+2r+2} + \frac{2(n-2)}{n+2r+3}\right) + \left(\frac{4r}{r+3} + \frac{2(n-2)r}{r+4}\right) + \left(\frac{2}{2r+4} + \frac{2(n-2)}{2r+5}\right) + \left(\frac{2}{2r+4} + \frac{2(n-2)}{2r+5}\right) + \frac{2(n-1)r}{r+3}.$$ □

Corollary 3. $H(\tilde{F}_n) = \frac{4}{n+2} + \frac{2(n-2)}{n+3} + 1 + \frac{4(n-2)}{5}$.

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

Proof. Let $C_n = v_1 v_2 \ldots v_n$ 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 ofharmonic index, we get

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

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$$=\frac{2r}{n+r+1}+\frac{2n}{n+2r+3}+\frac{2nr}{r+4}+\frac{2n}{2r+5}+\frac{2n}{2r+5}+\frac{2nr}{r+3}.\square$$

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

2. ZEROTH-ORDER GENERAL RANDICINDEX

Using the notations defined in above section, and combining with the definitions ofzeroth-order general Randic index, we get the following computational formulas.

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

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

$$\chi_\alpha(F_n)=n^\alpha+2^{\alpha+1}+(n-2)\cdot 3^\alpha.$$

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

$$=(n+r)^\alpha+n(3+r)^\alpha+r(n+1).$$

$$\chi_\alpha(W_n)=n^\alpha+n\cdot 3^\alpha.$$

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

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

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

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

$$\chi_\alpha(\tilde{F}_n)=n^\alpha+(n-2)\cdot 3^\alpha+(n+1)\cdot 2^\alpha.$$

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

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

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

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

$$\chi_{\alpha}(\tilde{W}_n)=n^{\alpha}+n\cdot 3^{\alpha}+n\cdot 2^{\alpha}.$$

3. CO-PI INDEX

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

Theorem 5. $Co-PI_v(I_r(F_n))=r^2(n+1)^2+r(2n^2-3n+3)+(n^2-3n+4)$.

Proof. Using the definition of Co-PI index, we have

$$Co-PI_v(I_r(F_n)) = \sum_{i=1}^{r}\left|n_v(vv^i)-n_{v^i}(vv^i)\right| + \sum_{i=1}^{n}\left|n_v(vv_i)-n_{v_i}(vv_i)\right| + \sum_{i=1}^{n-1}\left|n_{v_i}(v_iv_{i+1})-n_{v_{i+1}}(v_iv_{i+1})\right| +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}\left|n_{v_i}(v_iv_i^j)-n_{v_i^j}(v_iv_i^j)\right|$$

$$=r\left|(r+n(r+1))-1\right|+(2\left|(n-1)(r+1)-(r+1)\right|+(n-2)\left|(n-2)(r+1)-(r+1)\right|)$$

$$+2\left|2(r+1)-(r+1)\right|+(n-3)\left|2(r+1)-2(r+1)\right|+nr\left|(r+n(r+1))-1\right|$$

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

$$=r^2(n+1)^2+r(2n^2-3n+3)+(n^2-3n+4).\ \square$$

Corollary 5. $Co-PI_v(F_n)=n^2-3n+4$.

Theorem 6. $Co-PI_v(I_r(W_n))=r^2(n+1)^2+r(2n^2-3n-1)+(n^2-3n)$.

Proof. In view of the definition ofCo-PI index, we infer

$$Co-PI_v(I_r(W_n)) = \sum_{i=1}^{r}\left|n_v(vv^i)-n_{v^i}(vv^i)\right| + \sum_{i=1}^{n}\left|n_v(vv_i)-n_{v_i}(vv_i)\right| + \sum_{i=1}^{n}\left|n_{v_i}(v_iv_{i+1})-n_{v_{i+1}}(v_iv_{i+1})\right| +$$

$$\sum_{i=1}^{n}\sum_{j=1}^{r}\left|n_{v_i}(v_iv_i^j)-n_{v_i^j}(v_iv_i^j)\right|$$

$$=r\left|(r+n(r+1))-1\right|+n\left|(n-2)(r+1)-(r+1)\right|+n\left|2(1+r)-2(1+r)\right|+nr\left|(r+n(r+1))-1\right|$$

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

$$=r^2(n+1)^2+r(2n^2-3n-1)+(n^2-3n).\square$$

Corollary 6. $Co-PI_v(W_n)=n^2-3n$.

Theorem 7. $Co-PI_v(I_r(\tilde{F}_n))=4r^2n^2+r(22n^2-54n+32)+(18n^2-50n+32)$.

Proof. By virtue ofthe definition ofCo-PI index, we yield

$$Co-PI_v(I_r(\tilde{F}_n))=\sum_{i=1}^{r}\left|n_v(vv^i)-n_{v^i}(vv^i)\right|+\sum_{i=1}^{n}\left|n_v(vv_i)-n_{v_i}(vv_i)\right|+\sum_{i=1}^{n}\sum_{j=1}^{r}\left|n_{v_i}(v_iv_i^j)-n_{v_i^j}(v_iv_i^j)\right|$$

$$+\sum_{i=1}^{n-1}\left|n_{v_i}(v_iv_{i,i+1})-n_{v_{i,i+1}}(v_iv_{i,i+1})\right|+\sum_{i=1}^{n-1}\left|n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})-n_{v_{i+1}}(v_{i,i+1}v_{i+1})\right|$$

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

$$=r\left|r+(r+1)(2n-1)-1\right|+2\left|2(n-1)(r+1)-2(r+1)\right|+(n-2)\left|3(2n-3)(r+1)-(r+1)\right|+nr\left|2n(r+1)-2\right|$$

$$+(n-1)\left|3(2n-3)(r+1)-(r+1)\right|+(n-1)\left|3(2n-3)(r+1)-(r+1)\right|+(n-1)r\left|2n(r+1)-2\right|$$

$$=r(2nr+2n-2)+4(n-2)(r+1)+(n-2)(6n-10)(r+1)+nr(2nr+2n-2)+(n-1)(6n-10)(r+1)+$$

$$(n-1)(6n-10)(r+1)+(n-1)r(2nr+2n-2)$$

$$=4r^2n^2+r(22n^2-54n+32)+(18n^2-50n+32).\qquad\square$$

Corollary7. $Co-PI_v(\tilde{F}_n)=18n^2-50n+32$.

Theorem 8. $Co-PI_v(I_r(\tilde{W}_n))=r^2(2n^2+1)^2+r(22n^2-21n-1)+(18n^2-21n)$.

Proof. In view of the definition ofCo-PI index, we deduce

$$Co-PI_v(I_r(\tilde{W}_n))=\sum_{i=1}^{r}\left|n_v(vv^i)-n_{v^i}(vv^i)\right|+\sum_{i=1}^{n}\left|n_v(vv_i)-n_{v_i}(vv_i)\right|+\sum_{i=1}^{n}\sum_{j=1}^{r}\left|n_{v_i}(v_iv_i^j)-n_{v_i^j}(v_iv_i^j)\right|$$

$$+\sum_{i=1}^{n}\left|n_{v_i}(v_iv_{i,i+1})-n_{v_{i,i+1}}(v_iv_{i,i+1})\right|+\sum_{i=1}^{n}\left|n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})-n_{v_{i+1}}(v_{i,i+1}v_{i+1})\right|$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\left|n_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)-n_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j)\right|$$

$$=r\left|r+2n(r+1)-1\right|+n\left|3(2n-2)(r+1)-(r+1)\right|+nr\left|r+2n(r+1)-1\right|$$

$$+n\left|3(2n-2)(r+1)-(r+1)\right|+n\left|3(2n-2)(r+1)-(r+1)\right|+nr\left|(2n+1)(r+1)-2\right|$$

$$=r^2(2n^2+1)^2+r(22n^2-21n-1)+(18n^2-21n).\quad \square$$

Corollary 8. $Co-PI_v(\tilde{W}_n)=18n^2-21n$.

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