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RANDIC INDEX AND EDGE ECCENTRIC CONNECTIVITY INDEX OF CERTAIN SPECIAL MOLECULAR GRAPHS

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ABSTRACT

In this paper, we determine the Randic index and edge eccentric connectivity index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs.

Keywords: Chemical graph theory, Randic index, Edge eccentric connectivity index, Fan molecular graph, Wheel molecular graph, Gear fan molecular graph, Gear wheel molecular graph, *r*-corona molecular graph.

1. INTRODUCTION

Wiener index,edge Wiener index, Hyper-wiener index, Randic indexand edge eccentric connectivity indexare introduced to reflect certain structural features of organic molecules. Several papers contributed to determine the Wiener index or Hyper-wiener index of special molecular graphs (See Yan, et al. [1], Gao and Shi [2] and Yan, et al. [3] for more detail). 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 1975, Randic [4] introduced the Randic index as the sum of $d(u)d(v)^{-1/2}$ over all edges uv of a molecular graph G=(V, E), i.e.

$$R(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}$$

Where$d(u)$ denotes the degree of $u \in V(G)$. Later in 1998, Bollobas and Erdos [5] generalized this index by replacing −1/2 with any real number α , which is called the general Randic index, i.e.

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

Li and Liu [6] determined the first three minimum general Randic indices among trees, and the corresponding extremal trees are characterized. Liu, et al. [7] gave a best-possible lower bound on the Randic index of a triangle-free molecular graph *G* with given minimum degree $\delta(G) \geq 2$. Yang and Lu [8] presented the relationship between Randic indices and the diameter of molecular graph. Liu, et al. [9] presented a upper bound on the Randic index for all chemical molecular graphs with n vertices, $m \geq n$ edges and $k > 0$ pendant vertices, and determined corresponding extremal molecular graphs. Yero and Velazquez [10] obtained the lower and upper bounds of Randic index for some corona product molecular graphs. Yu and Feng [11] considered the relationship between Randic index and the eigenvalues of molecular graphs. Liu, et al. [12] determined a sharp lower bound on the Randic index of unicyclic molecular graphs in terms of the order and given size of matching.

Let $f = uv$ be an edge in $E(G)$. Then the degree of the edge f is defined to be $\deg_G(u) + \deg_G(v) - 2$. For two edges $f_1 = u_1v_1, f_2 = u_2v_2$ in $E(G)$, the distance between f_1 and f_2, denoted by $d_G(f_1, f_2)$, is defined to be

$$d_G(f_1, f_2) = \min\{d_G(u_1,u_2), d_G(u_1,v_2), d_G(v_1,u_2), d_G(v_1,v_2)\}.$$

The eccentricity of an edge f, denoted by $ec_G(f)$, is defined as

$$ec_G(f) = \max\{d_G(f,e) \mid e \in E(G)\}.$$

The edge eccentric connectivity index of *G*, denoted by $\xi_e^c(G)$, is defined as

$$\xi_e^c(G) = \sum_{f \in E(G)} \deg_G(f) ec_G(f).$$

Xu and Guo [13] obtained various upper and lower bounds for this index of connected molecular graphs in terms of order, size, girth and the first Zagreb index of *G*, respectively. Other results on edge eccentric connectivity index can refer to Odabaş [14].

In this paper, we present the Randic indexof $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$. Also, the edge eccentric connectivity index of $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$ are derived.

2. RANDIC INDEX

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

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 ($1\leq i\leq n$). 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 Randic index, we have

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

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

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

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

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 ($1\leq i\leq n$). 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 Randic index, we have

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

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

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

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

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

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 ofthe definition of Randic index, we get

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

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

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

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

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

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

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 Randic index, we deduce

$$R(I_r(\tilde{W}_n)) = \sum_{i=1}^{r}(d(v)d(v^i))^{-1/2} + \sum_{i=1}^{n}(d(v)d(v_i))^{-1/2} + \sum_{i=1}^{n}\sum_{j=1}^{r}(d(v_i)d(v_i^j))^{-1/2} +$$

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

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

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

3. EDGE ECCENTRIC CONNECTIVITY INDEX

Theorem 5. $\xi_e^c(I_r(F_n))=n^2+n(2r^2+11r+9)+r^2-9r-14$.

Proof. By the definition of edge eccentric connectivity index, we have

$$\xi_e^c(I_r(F_n))=\sum_{i=1}^{r}\deg_G(vv^i)ec_G(vv^i)+\sum_{i=1}^{n}\deg_G(vv_i)ec_G(vv_i)+\sum_{i=1}^{n-1}\deg_G(v_iv_{i+1})ec_G(v_iv_{i+1})$$

$$+\sum_{i=1}^{n}\sum_{j=1}^{r}\deg_G(v_iv_i^j)ec_G(v_iv_i^j)$$

$$=r(n+r-1)+(2(n+2r)+(n-2)(n+2r+1))+(2\times2(2r+3)+(n-3)\times2(2r+4))+r(2\times2(r+1)+(n-2)\times2(r+2))$$

$$=n^2+n(2r^2+11r+9)+r^2-9r-14.$$

Corollary 5. $\xi_e^c(F_n)=n^2+9n-14$.

Theorem 6. $\xi_e^c(I_r(W_n))=n^2+n(2r^2+11r+9)+r^2-r$.

Proof. By the definition of edge eccentric connectivity index, we have

$$\xi_e^c(I_r(W_n))=\sum_{i=1}^{r}\deg_G(vv^i)ec_G(vv^i)+\sum_{i=1}^{n}\deg_G(vv_i)ec_G(vv_i)+$$

$$\sum_{i=1}^{n}\deg_G(v_iv_{i+1})ec_G(v_iv_{i+1})+\sum_{i=1}^{n}\sum_{j=1}^{r}\deg_G(v_iv_i^j)ec_G(v_iv_i^j)$$

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

$$=n^2+n(2r^2+11r+9)+r^2-r.$$

Corollary 6. $\xi_e^c(W_n)=n^2+9n$.

Theorem 7. $\xi_e^c(I_r(\tilde{F}_n))=2n^2+n(7r^2+28r+20)-2r^2-24r-28$.

Proof. By virtue ofthe definition of edge eccentric connectivity index, we get

$$\xi_e^c(I_r(\tilde{F}_n)) = \sum_{i=1}^{r}\deg_G(vv^i)ec_G(vv^i) + \sum_{i=1}^{n}\deg_G(vv_i)ec_G(vv_i) + \sum_{i=1}^{n}\sum_{j=1}^{r}\deg_G(v_iv_i^j)ec_G(v_iv_i^j) + \sum_{i=1}^{n-1}\deg_G(v_iv_{i,i+1})ec_G(v_iv_{i,i+1}) + \sum_{i=1}^{n-1}\deg_G(v_{i,i+1}v_{i+1})ec_G(v_{i,i+1}v_{i+1}) + \sum_{i=1}^{n-1}\sum_{j=1}^{r}\deg_G(v_{i,i+1}v_{i,i+1}^j)ec_G(v_{i,i+1}v_{i,i+1}^j)$$

$$= 2r(n+r-1) + (2\times 2(n+2r)+(n-2)\times 2(n+2r+1)) + r(2\times 3(r+1)+(n-2)\times 3(r+2)) + (3(2r+2)+(n-2)\times 3(2r+3)) + (3(2r+2)+(n-2)\times 3(2r+3)) + (n-1)4r(r+1)$$

$$= 2n^2 + n(7r^2+28r+20) - 2r^2 - 24r - 28.$$

Corollary 7. $\xi_e^c(\tilde{F}_n) = n^2 + 13n - 18$.

Theorem 8. $\xi_e^c(I_r(\tilde{W}_n)) = 2n^2 + n(7r^2+28r+20) + 2r^2 - 2r$.

Proof. In view of the definition of edge eccentric connectivity index, we deduce

$$\xi_e^c(I_r(\tilde{W}_n)) = \sum_{i=1}^{r}\deg_G(vv^i)ec_G(vv^i) + \sum_{i=1}^{n}\deg_G(vv_i)ec_G(vv_i) + \sum_{i=1}^{n}\sum_{j=1}^{r}\deg_G(v_iv_i^j)ec_G(v_iv_i^j) + \sum_{i=1}^{n}\deg_G(v_iv_{i,i+1})ec_G(v_iv_{i,i+1}) + \sum_{i=1}^{n}\deg_G(v_{i,i+1}v_{i+1})ec_G(v_{i,i+1}v_{i+1}) + \sum_{i=1}^{n}\sum_{j=1}^{r}\deg_G(v_{i,i+1}v_{i,i+1}^j)ec_G(v_{i,i+1}v_{i,i+1}^j)$$

$$= 2r(n+r-1) + 2n(n+2r+1) + 3nr(r+2) + 3n(2r+3) + 3n(2r+3) + 4nr(r+1)$$

$$= 2n^2 + n(7r^2+28r+20) + 2r^2 - 2r.$$

Corollary 8. $\xi_e^c(\tilde{W}_n) = n^2 + 13n$.

4. CONCLUSION AND DISCUSSION

In this paper, we determine the Randic index and edge eccentric connectivity index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their *r*-corona molecular graphs. The Hosoya index $Z(G)$ of molecular graph G is defined as the number of subsets of the edge set $E(G)$ in which no two edges are adjacent in G, i.e., $Z(G)$ is the total number of matchings of G. Hence, the Hosoya index of a molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their *r*-corona molecular graphs should considered as our further work.

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