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RESULTS ON GENERALIZED HARARY INDEX AND ECCENTRIC CONNECTIVITY POLYNOMIAL

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Abstract:-

Chemical compounds and drugs are often modeled as graphs where each vertex represents an atom of molecule and covalent bounds between atoms are represented by edges between the corresponding vertices. This graph derived from a chemical compounds is often called its molecular graph and can be different structures. In this paper, we determine the accurate formulas to compute the generalized Harary index and eccentric connectivity polynomial of certain special molecular graphs.

Keywords:-Molecular graph; generalized Harary Index; eccentric connectivity polynomial

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1. INTRODUCTION

Wiener index, Harary index, Shultz index, Geometric-arithmetic index and degree distance are introduced to reflect certain structural features of organic molecules. Several papers contributed to determine the distance-based index or degree-based index of special molecular graphs (See Yan et al., [1-2], Gao et al., [3-4], Gao and Shi [5], Gao and Wang [6], Xi and Gao [7-8], Xi et al., [9], Gao et al., [10] for more detail). The notation and terminology used but undefined in this paper can be found in [11]. In what follows, we only consider simple and connected molecular graph.

We denote P_n and C_n are path and cycle with n vertices. The graph $F_n = \{v\} \Box P_n$ is called a fan graph and the graph $W_n = \{v\}$ $\Box C_n$ is called a wheel graph. Graph $I_r(G)$ is called r- crown 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 graph F_n , the resulting graph is a subdivision graph called gear fan graph, denote as F_n . By adding one vertex in every two adjacent vertices of the wheel cycle C_n of wheel graph W_n , The resulting graph is a subdivision graph, called gear wheel graph, denoted as W_n .

The the second Harary index and the third Harary index was introduced by Das et al., [12]:

$$
H_1(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)+1},
$$

And

$$
H_2(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v)+2}
$$

As an extension, they defined the generalized Harary index as:

$$
H_t(G) = \sum_{\{u,v\} \subseteq V(G)} \frac{1}{d(u,v) + t},
$$

Where *it* is any non-negative real number.

The eccentric connectivity polynomial was defined as

$$
\zeta^{c}(G,x)=\sum_{v\in V(G)}d(v)x^{ec(v)},
$$

Where eccentricity ec (u) of vertex $u \Box V(G)$ is the maximum distance between u and any other vertex in G_{∞}

In this paper, we first present the generalized Harary index of $IF_r(n)$, $I W_r(n)$ $I_r(F_n)$ and $I W_r(n)$. Then, We determine the eccentric connectivity polynomial of these molecular graphs.

2. Main results and proof 2.1 Generalized Harary index

Theorem 1.
$$
H_t(I_r(F_n)) = \left(\frac{3n^2 - 3n + 3}{3 + t} + \frac{2n^2 + 2}{2 + t} + \frac{2n}{1 + t}\right)r^2 + \left(\frac{12n^2 - 26n + 16}{3 + t}\right)
$$

+ $\frac{2n^2 + 2n + 4}{2 + t} + \frac{11n - 3}{1 + t}r + \left(\frac{n^2 + 3n - 2}{1 + t} + \frac{3n^2 - 8n + 15}{2 + t}\right)$.

Proof. Let $P_n = v_1v_2...v_n$ 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' . By the definition of generalized Harary index, we have

$$
H_{t}(I_{r}(F_{s})) = \sum_{i=1}^{r-1} \sum_{j=i}^{r} \frac{1}{d(v_{i},v^{j})+t} + \sum_{i=1}^{r} \frac{1}{d(v_{i},v^{j})+t} + \sum_{i=1}^{n} \frac{1}{d(v_{i},v_{i})+t} + \sum_{i=1}^{n} \sum_{j=i}^{r} \frac{1}{d(v_{i},v_{j})+t} + \sum_{i=1}^{n-1} \sum_{j=i}^{r} \sum_{k=i}^{r} \frac{1}{d(v_{i},v^{j})+t} + \sum_{i=1}^{n-1} \sum_{j=i+1}^{r} \sum_{k=i}^{r} \frac{1}{d(v_{i},v^{j})+t} + \sum_{i=1}^{n-1} \sum_{j=i+1}^{r} \sum_{k=i}^{r} \sum_{j=i+1}^{r} \frac{1}{d(v_{i},v^{j})+t} + \sum_{j=i+1}^{r} \
$$

Theorem 2,
$$
H_i(I_r(W_n)) = \left(\frac{n^2 - \frac{3}{2}n}{4 + t} + \frac{2n}{3 + t} + \frac{3n + 1}{2 + t} + \frac{n + 1}{1 + t}\right)r^2 + \left(\frac{3n^2 - 5n}{3 + t} + \frac{2n^2 + 2n - 1}{2 + t} + \frac{7n + 1}{1 + t}\right)r + \left(\frac{12n^2 - 20n}{3 + t} + \frac{3n^2 - 6n}{2 + t} + \frac{n^2 + 3n}{1 + t}\right).
$$

Proof. Let $C_n = v_1v_2...v_n$ and $v_1^1, v_2^2,..., v_n^r$ 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 generalized Harary index, we deduce

$$
H_i(I_r(W_n)) = \sum_{i=1}^{r-1} \sum_{j=i}^{r} \frac{1}{d(v^i, v^j) + t} + \sum_{i=1}^{r} \frac{1}{d(v, v^i) + t} + \sum_{i=1}^{n} \frac{1}{d(v, v_i) + t} + \sum_{i=1}^{n} \sum_{j=1}^{r} \frac{1}{d(v, v^j) + t} +
$$

$$
\sum_{i=1}^{n} \sum_{j=1}^{r} \frac{1}{d(v_i, v^i) + t} + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{k=1}^{r} \frac{1}{d(v_i^i, v^k) + t} + \sum_{i=1}^{r-1} \sum_{j=i+1}^{s} \frac{1}{d(v_i, v_j) + t} + \sum_{i=1}^{r} \sum_{j=i+1}^{s} \frac{1}{d(v_i^i, v^k) + t} + \sum_{i=1}^{r-1} \sum_{j=i+1}^{s} \sum_{k=i+1}^{r} \frac{1}{d(v_i^i, v^k) + t} + \sum_{i=1}^{r-1} \sum_{j=i+1}^{s} \sum_{k=i+1}^{r} \frac{1}{d(v_i^i, v^k) + t} + \sum_{i=1}^{r-1} \sum_{j=i+1}^{r} \sum_{k=i+1}^{r} \frac{1}{d(v_i^i, v^k) + t} + \sum_{i=1}^{r} \sum_{j=i+1}^{r} \sum_{k=i+1}^{r} \frac{1}{d(v_i^i, v^k) + t} + \sum_{i=1}^{r} \sum_{j=i+1}^{r} \sum_{j
$$

 $\qquad \qquad +(\frac{n^2+3n-2}{1+t}+\frac{6n^2-6n}{2+t}+\frac{15n^2-41n+30}{3+t}+\frac{4n^2-10n+7}{4+t})\ .$ **Proof.** Let $P_n = v_1v_2...v_n$ and $v_{i,j+1}$ 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'. By virtue of the definition of generalized Harary index we a

$$
H_{i}(I_{i}(\tilde{F}_{n})) = \sum_{i=1}^{n} \sum_{j=1}^{r} \frac{1}{d(v_{i},v^{j})+t} + \sum_{i=1}^{r} \frac{1}{d(v_{i},v^{j})+t} + \sum_{i=1}^{n} \frac{1}{d(v_{i},v_{j})+t} + \sum_{i=1}^{n} \sum_{j=1}^{r} \frac{1}{d(v_{i},v^{j})+t} + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{k=1}^{r} \frac{1}{d(v^{j},v^{j})+t} + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{k=1}^{r} \frac{1}{d
$$

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$$
\sum_{i=1}^{n-1} \sum_{j=1}^{n} \sum_{k=j+i}^{r} \frac{1}{d(v_{i_{j+1}}^j, v_{i_{j+1}}^j) + t} + \sum_{i=1}^{n-2} \sum_{j=i+1}^{n-1} \sum_{k=i}^{r} \sum_{j=i+1}^{r} \frac{1}{d(v_{i_{j+1}}^j, v_{i_{j+1}}^j) + t}
$$
\n
$$
= \frac{r(r-1)}{2+t} + \frac{r(n+r+1)}{1+t} + \frac{2nr + n^2 + 3n - 2}{1+t} + \frac{nr(n+r+1)}{2+t} + \frac{r^2n + r(4n-2)}{2+t} + \frac{2nr^2}{3+t} + \frac{r(n^2-n) + r(12n^2 - 18n + 6)}{3+t} + \frac{nr(r-1)}{2+t} + \frac{r^2(n-1)}{4+t} + \frac{r(n-1)(n+2r+2)}{4+t} + \frac{r(n-1)(n+r+1)}{3+t} + \frac{r(n-1)(r+3)}{2+t} + \frac{r^2(n-1)}{2+t} + \frac{r(6n^2 - 14n + 8) + (15n^2 - 41n + 30)}{3+t} + \frac{r(n^2 - 2n + 1) + (4n^2 - 10n + 7)}{4+t} + \frac{(r^2 + 3r)(n-1)^2}{4+t} + \frac{2r^2(5n-4)(n-1)}{5+t} + \frac{(r+2)(n-2)^2}{2+t} + \frac{(r^2+3r)(n-1)}{1+t} + \frac{(r^2+3r)(5n^2-19n+18)}{5+t} + \frac{r(n-1)(r-1)}{1+t} + \frac{(3n-6)(3n-5)r^2}{2+t} + \frac{(3n^2 - n+1)}{4+t} + \frac{15n^2 - 37n + 26}{5+t} + \frac{9n^2 - 33n + 30}{6+t} + \frac{r^2}{6+t} + \frac{r^2(n-1)(n+1)}{5+t} + \frac{(n^2+3n-2)(n+1)}{1+t} + \frac{(n^2+3n-2)(n+1)}{1+t} + \frac{(n^2+3n-2)(n+1)}{1+t} + \frac{(n^2+3n-2)(n+1)}
$$

Proof. Let $C_e = v_1v_2...v_n$ and v be a vertex in W_e beside C_e . Let $V_{e,e+1}$ \cup 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 $v_{n,n+1} = v_{i,n}$ 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 generalized Harary index, we yield

$$
H_{i}(I_{r}(\vec{W}_{n})) = \sum_{|\alpha|}\sum_{j=1}^{r-1}\sum_{d(\gamma_{j},\gamma_{j})+t}^{r} + \sum_{j=1}^{r}\frac{1}{d(\gamma_{j},\gamma_{j})+t} + \sum_{i=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r}\frac{1}{d(\gamma_{i},\gamma_{j})+t} + \sum_{i=1}^{r}\sum_{j=1}^{r}\sum_{k=1}^{r
$$

Corollary 4.
$$
H_t(\tilde{W}_u) = \frac{n^2 + 3n}{1+t} + \frac{4n^2 - n}{2+t} + \frac{2n^2 - 4n}{4+t}
$$
.

2.2 Eccentric connectivity polynomial

Theorem 5. $\xi^*(I_r(F_n), x) = (r+n)x^2 + (nr+(3n-2)+r)x^3 + mrx^4$.

Proof. By the definition of eccentric connectivity polynomial, we have

$$
\zeta^{\epsilon}(I_{r}(F_{s}), x) = \deg(v)x^{\epsilon(\nu)} + \sum_{i=1}^{n} \deg(v_{i})x^{\epsilon(\nu_{i})} + \sum_{i=1}^{r} \deg(v^{i})x^{\epsilon(\nu^{i})} + \sum_{i=1}^{n} \sum_{j=1}^{r} \deg(v^{j})x^{\epsilon(\nu^{j})}
$$

= $(r+n)x^{2} + (nr + (3n-2))x^{3} + rx^{4} + nrx^{4} = (r+n)x^{2} + (nr + (3n-2) + r)x^{3} + nrx^{4}$.
Corollary 5 $\zeta^{\epsilon}(F_{s}, x) = nx^{2} + (3n-2)x^{3}$.

Theorem 6. $\xi^* (I_1(W_1), x) = (r+n)x^2 + (nr+3n+r)x^3 + nrx^4$. Proof. By the definition of eccentric connectivity polynomial, we have

$$
\zeta^{2} (I_{r}(W_{n}), x) = \deg(v) x^{\alpha(v)} + \sum_{i=1}^{n} \deg(v_{i}) x^{\alpha(v_{i})} + \sum_{i=1}^{r} \deg(v^{i}) x^{\alpha(v^{i})} + \sum_{i=1}^{n} \sum_{j=1}^{r} \deg(v^{j}) x^{\alpha(v^{j})}
$$

= $(r+n)x^{2} + (nr+3n)x^{3} + rx^{3} + mx^{4} = (r+n)x^{2} + (nr+3n+r)x^{3} + mrx^{4}$.
Corollary 6. $\zeta^{2} (W_{n}, x) = nx^{2} + 3nx^{3}$.

Theorem 7. $\xi^* (I_n(\tilde{F}_n), x) = (r+n)x^3 + ((n+1)r + (3n-2))x^4 + ((n-1)(2+r) + nr)x^5 + r(n-1)x^6$. Proof. By virtue of the definition of eccentric connectivity polynomial, we get

$$
\zeta^{*}(I,(\tilde{F}_{n}),x) = \deg(v)x^{m(v)} + \sum_{i=1}^{n} \deg(v_{i})x^{m(v)} + \sum_{i=1}^{n} \deg(v^{i})x^{m(v)} + \sum_{i=1}^{n} \sum_{j=1}^{n} \deg(v_{j})x^{m(v)} + \sum_{i=1}^{n-1} \deg(v_{i+1})x^{m(v)} + \sum_{i=1}^{n-1} \sum_{j=1}^{n} \deg(v_{i+1})x^{m(v_{i+1})}
$$
\n
$$
= (r+n)x^{3} + (nr+(3n-2))x^{4} + rx^{4} + nrx^{5} + (n-1)(2+r)x^{5} + r(n-1)x^{6}
$$
\n
$$
= (r+n)x^{3} + ((n+1)r + (3n-2))x^{4} + ((n-1)(2+r) + nr)x^{5} + r(n-1)x^{6}.
$$
\nCorollary 7.
$$
\zeta^{*}(\tilde{F}_{n},x) = nx^{3} + (3n-2)x^{4} + 2(n-1)x^{5}.
$$

Theorem 8. $\xi^*(I_n(\vec{W}_n), x) = (r+n)x^4 + (nr+3n+r)x^4 + (2n+2nr)x^5 + nrx^6$. Proof. In view of the definition of eccentric connectivity polynomial, we deduce

$$
\xi^{\epsilon}(I_{\epsilon}(\tilde{W}_{\epsilon}),x) = \deg(v)x^{\epsilon(\epsilon_{1})} + \sum_{i=1}^{n} \deg(v_{i})x^{\epsilon(\epsilon_{2})} + \sum_{i=1}^{r} \deg(v^{i})x^{\epsilon(\epsilon_{2}^{i})} + \sum_{i=1}^{n} \sum_{j=1}^{r} \deg(v^{j}_{j})x^{\epsilon(\epsilon_{2}^{j})} + \sum_{i=1}^{n} \deg(v_{i,i+1}^{j})x^{\epsilon(\epsilon_{2}^{j})} + \sum_{i=1}^{n-1} \sum_{j=1}^{r} \deg(v_{i,i+1}^{j})x^{\epsilon(\epsilon_{2}^{j})} + \sum_{i=1}^{n-1} \sum_{j=1}^{r} \deg(v_{i,i+1}^{j})x^{\epsilon(\epsilon_{2}^{j})} + \sum_{i=1}^{n} \deg(v_{i,i+1}^{j})x^
$$

3. Conclusion

In this paper, we present the generalized Harary index and eccentric connectivity polynomial of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs. The results obtained in our paper illustrate the promising application prospects for chemistry and pharmacy science.

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