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Minimum Hyper-Wiener Index of Molecular Graph and Some Results on Szeged Related Index

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***Abstract*—Hyper-Wiener index, edge-vertex Szeged index and vertex-edge Szeged index are important topological indices in theoretical chemical. In this paper, we first determine the minimum Hyper-Wiener index of graph with connectivity or edge-connectivity. Then, the edge-vertex Szeged index and vertex-edge Szeged index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their *r*-corona molecular graphs are presented.**

Keywords—Chemical graph theory, organic molecules, Hyper-Wiener index, connectivity, edge-connectivity, edge-vertex Szeged index, vertex-edge Szeged index

I. INTRODUCTION

Hyper-Wiener index, edge-vertex Szeged index and vertex-edge Szeged index are introduced to reflect certain structural features of organic molecules. Several papers contributed to determine the distance-based index of special molecular graphs (See Yan et al., [1] and [2], Gao and Shi [3], Gao and Gao [4] and [5], and Xi and Gao [6] 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 $\tilde{W}_n$.

The Hyper-Wiener index WW is one of the recently distance-based graph invariants. That WW clearly encodes the compactness of a structure and the WW of G is define as:

$$WW(G)=\frac{1}{2}\left(\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2+\sum_{\{u,v\}\subseteq V(G)} d(u,v)\right).$$

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 the distance 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. The number of edges of G whose distance to the vertex u is smaller than the distance to the vertex v is denoted by $m_u(e)$. Analogously, $m_v(e)$ is the number of edges of G whose distance to the vertex v is smaller than the distance to the vertex u. The edge-vertex Szeged index and vertex-edge Szeged index are defined as follows:

$$Sz_{ev}(G)=\frac{1}{2}\sum_{e=uv}(m_u(e)n_v(e)+m_v(e)n_u(e)),$$

$$Sz_{ve}(G)=\frac{1}{2}\sum_{e=uv}(m_u(e)n_u(e)+m_v(e)n_v(e)).$$

Some conclusions on edge-vertex Szeged index and vertex-edge Szeged index can refer to [7].

In this paper, we first determine the minimum Hyper-Wiener index of graph with connectivity or edge-connectivity, then present the edge-vertex Szeged index and vertex-edge Szeged index of $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$.

II. MAIN RESULTS AND PROOFS

Let G be a connected graph on n vertices. It is clear that the Hyper-Wiener index is minimal if and only if $G=K_n$, in which case, $W(G)=WW(G)=\frac{n(n-1)}{2}$. In what follows, we investigate when a graph with a given vertex or edge-connectivity has minimum Hyper -Wiener index.

Theorem 1. Let G be a k-connected, n-vertex graph, $1\le k\le n-2$. Then

$$WW(G)\ge\frac{n(n-1)}{2}+2(n-k-1).$$

Equality holds if and only if $G=K_k \vee (K_1 \cup K_{n-k-1})$.

Proof. Let $G_{\min}$ be the graph that among all graphs on n vertices and connectivity k has minimum Hyper-Wiener index. Since the connectivity of $G_{\min}$ is k, there is a vertex-cut $X \subset V(G_{\min})$, such that $|X|=k$. Denote the components of $G_{\min}-X$ by $G_1, G_2, \ldots, G_\omega$. Then each of the sub-graphs $G_1, G_2, \ldots, G_\omega$ must be complete. Otherwise, if one of them would not be complete, then by adding an edge between two nonadjacent vertices in this sub-graph we would arrive at a graph with the same number of vertices and same connectivity, but smaller Hyper-Wiener index, a contradiction.

It must be $\omega=2$. Otherwise, by adding an edge between a vertex from one component and a vertex from another component $G_1, G_2, \ldots, G_\omega$, if $\omega>2$, then the resulting graph would still have connectivity k, but its Hyper-Wiener index would decrease, a contradiction. Hence, $G_{\min}-X$ has two components G_1 and G_2. By a similar argument, we conclude that any vertex in G_1 and G_2 is adjacent to any vertex in X.

Denote the number of vertices of G_1 by n_1 and that of G_2 by n_2. Then $n_1+n_2+k=n$ and by direct calculation we get

$$WW(G_{\min}) = \frac{1}{2}\Big\{\Big\{\frac{1}{2}n_1(n_1-1)+\frac{1}{2}n_2(n_2-1)+\frac{1}{2}k(k-1)+k(n_1+n_2)+4n_1n_2\Big\}+\Big\{\frac{1}{2}n_1(n_1-1)+\frac{1}{2}n_2(n_2-1)+\frac{1}{2}k(k-1)+k(n_1+n_2)+2n_1n_2\Big\}\Big\}$$

which for fixed n and k is minimum for $n_1=1$ or $n_2=1$. This in turn means that $G_{\min}= K_k \vee (K_1 \cup K_{n-k-1})$. Direct calculation yields

$$WW(G_{\min}) = \frac{n(n-1)}{2}+2(n-k-1)$$

which completes the proof.

The edge-connectivity version for Theorem 1 is also valid. Here the case $k=n-1$ needs not be considered, since the only $(n-1)$-edge connected graph is K_n.

Theorem 2. Let G be a k-edge connected, n-vertex graph, $1 \le k \le n-2$. Then

$$WW(G) \ge \frac{n(n-1)}{2}+2(n-k-1).$$

Equality holds if and only if $G=K_k \vee (K_1 \cup K_{n-k-1})$.

Proof. Let now $G_{\min}$ denote the graph that among all graphs with n vertices and edge-connectivity k has minimum Hyper-Wiener index. Let X be an edge-cut of $G_{\min}$ with $|X|=k$. Then $G_{\min}-X$ has two components, G_1 and G_2. Both G_1 and G_2 must be complete graphs. Let $|V(G_1)|=n_1$ and $|V(G_2)| = n_2$, $n_1+ n_2= n$.

Denote the set of the end-vertices of the edges of X in G_1 by S, and that in G_2 by T. Let $|V(G_1-S)|=a_1$ and $|V(G_2-S)|=a_2$.

There are

$$\frac{1}{2}n_1(n_1-1)+\frac{1}{2}n_2(n_2-1)+k=|E(G_{\min})|$$

pairs of vertices at distance 1, and a_1a_2 pairs of vertices at distance of 3. All other vertex pairs, namely

$$\binom{n}{2}-|E(G_{\min})|-a_1a_2$$

are at distance 2. Consequently,

$$WW(G_{\min}) = \frac{1}{2}\Big\{\Big\{\Big[\frac{1}{2}n_1(n_1-1)+\frac{1}{2}n_2(n_2-1)+k\Big]+4\Big[\binom{n}{2}-\Big(\frac{1}{2}n_1(n_1-1)+\frac{1}{2}n_2(n_2-1)+k\Big)-a_1a_2\Big]+9[a_1a_2]\Big\}+\Big\{\Big[\frac{1}{2}n_1(n_1-1)+\frac{1}{2}n_2(n_2-1)+k\Big]+2\Big[\binom{n}{2}-\Big(\frac{1}{2}n_1(n_1-1)+\frac{1}{2}n_2(n_2-1)+k\Big)-a_1a_2\Big]+3[a_1a_2]\Big\}\Big\}$$

$$= \frac{1}{2}\Big\{\Big\{\frac{1}{2}n(n-1)-3k+3n_1n_2+5a_1a_2\Big\}+\Big\{\frac{1}{2}n(n-1)-k+n_1n_2+a_1a_2\Big\}\Big\}$$

$$= \frac{1}{2}n(n-1)-2k+2n_1n_2+3a_1a_2$$

which for fixed n and k is minimum for $n_1=1$, $a_1=0$ or $n_2=1$, $a_2=0$. This, as before, implies $G_{\min} = K_k \vee (K_1 \cup K_{n-k-1})$. Hence,

$$WW(G_{\min}) = \frac{n(n-1)}{2}+2(n-k-1).$$

Theorem 3. $Sz_{ev}(I_r(F_n)) = r^2(2n^2+4n-6)$

$+r(\frac{9}{2}n^2+4n-20)+(2n^2+\frac{3}{2}n-12)$.

Proof. Let $P_n=v_1v_2\dots v_n$ 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 edge-vertex Szeged index, we have

$Sz_{ev}(I_r(F_n))=$

$$\frac{1}{2}\sum_{i=1}^{r}\sum_{e=uv}(m_{v^i}(vv^i)n_v(vv^i)+m_v(vv^i)n_{v^i}(vv^i))+$$

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_i}(vv_i)n_v(vv_i)+m_v(vv_i)n_{v_i}(vv_i))$$

$$+\frac{1}{2}\sum_{i=1}^{n-1}\sum_{e=uv}(m_{v_{i+1}}(v_iv_{i+1})n_{v_i}(v_iv_{i+1})+m_{v_i}(v_iv_{i+1})n_{v_{i+1}}(v_iv_{i+1}))$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{e=uv}(m_{v_i^j}(v_iv_i^j)n_{v_i}(v_iv_i^j)+m_{v_i}(v_iv_i^j)n_{v_i^j}(v_iv_i^j))$$

$$=\frac{r}{2}[1\times(r+n(r+1))+(2n+r+nr-2)\times 1]$$

$$+\frac{1}{2}(2[(r+2)\times(n-1)(r+1)+(2n+nr-2r-4)\times(r+1)]$$
$$+(n-2)[(r+2)\times(n-2)(r+1)+(2n+nr-2r-5)\times(r+1)])$$
$$+\frac{1}{2}(2[(2r+3)\times(r+1)+(r+1)\times 2(r+1)]$$
$$+2[(2r+3)\times 2(r+1)+(2r+2)\times 2(r+1)]$$
$$+(n-5)[(2r+3)\times 2(r+1)+(2r+3)\times 2(r+1)])$$
$$+\frac{nr}{2}[1\times(r+n(r+1))+(2n+r+nr-2)\times 1]$$

$$=r^2(2n^2+4n-6)+r(\frac{9}{2}n^2+4n-20)+(2n^2+\frac{3}{2}n-12)$$

Corollary 1. $Sz_{ev}(F_n)=2n^2+\frac{3}{2}n-12$.

Theorem 4. $Sz_{ev}(I_r(W_n))=r^2(n^2+8n-3)$ $+r(\frac{3}{2}n^2+17n-\frac{27}{2})+(10n-9)$.

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 edge-vertex Szeged index, we infer

$Sz_{ev}(I_r(W_n))=$

$$\frac{1}{2}\sum_{i=1}^{r}\sum_{e=uv}(m_{v^i}(vv^i)n_v(vv^i)+m_v(vv^i)n_{v^i}(vv^i))$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_i}(vv_i)n_v(vv_i)+m_v(vv_i)n_{v_i}(vv_i))$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_{i+1}}(v_iv_{i+1})n_{v_i}(v_iv_{i+1})+m_{v_i}(v_iv_{i+1})n_{v_{i+1}}(v_iv_{i+1}))$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{e=uv}(m_{v_i^j}(v_iv_i^j)n_{v_i}(v_iv_i^j)+m_{v_i}(v_iv_i^j)n_{v_i^j}(v_iv_i^j))$$

$$=\frac{r}{2}[1\times(r+n(r+1))+(2n+r+nr-1)\times 1]$$

$$+\frac{n}{2}[(r+2)\times(n-2)(r+1)+(2n+nr-2r-5)\times(r+1)]+$$
$$\frac{n}{2}[(2r+3)\times 2(1+r)+(2r+3)\times 2(1+r)]$$

$$+\frac{nr}{2}[(2n+r+nr-1)\times 1+1\times(r+n(r+1))]$$

$$=r^2(n^2+8n-3)+r(\frac{3}{2}n^2+17n-\frac{27}{2})+(10n-9)$$

Corollary 2. $Sz_{ev}(W_n)=10n-9$.

Theorem 5. $Sz_{ev}(I_r(\tilde{F}_n))=r^2(22n^2-35n+20)$

$$+r(\frac{85}{2}n^2-\frac{179}{2}n+50)+(\frac{39}{2}n^2-\frac{101}{2}n+30).$$

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 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 of the definition of edge-vertex Szeged index, we yield

$Sz_{ev}(I_r(\tilde{F}_n))=$

$\frac{1}{2}\sum_{i=1}^{r}\sum_{e=uv}(m_{v^i}(vv^i)n_v(vv^i)+m_v(vv^i)n_{v^i}(vv^i))$ +

$\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_i}(vv_i)n_v(vv_i)+m_v(vv_i)n_{v_i}(vv_i))$

+

$\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{e=uv}(m_{v_i^j}(v_iv_i^j)n_{v_i}(v_iv_i^j)+m_{v_i}(v_iv_i^j)n_{v_i^j}(v_iv_i^j))$

+

$\frac{1}{2}\sum_{i=1}^{n-1}(m_{v_{i,i+1}}(v_iv_{i,i+1})n_{v_i}(v_iv_{i,i+1})+m_{v_i}(v_iv_{i,i+1})n_{v_{i,i+1}}(v_iv_{i,i+1}))$

+

$\frac{1}{2}\sum_{i=1}^{n-1}(m_{v_{i+1}}(v_{i,i+1}v_{i+1})n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})+m_{v_{i,i+1}}(v_{i,i+1}v_{i+1})n_{v_{i+1}}(v_{i,i+1}v_{i+1}))$

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

$+m_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)n_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j))$

$=\frac{r}{2}[(3n+2nr-3)\times1+1\times(r+(r+1)(2n-1)]$

+

$\frac{1}{2}(2[(2r+1)\times(2n-2)(r+1)+(2nr+3n-2r-5)\times2(r+1)]$

+

$(n-2)[(3r+2)\times(2n-3)(r+1)+(2nr+3n-3r-7)\times3(r+1)])$

+ $\frac{nr}{2}[1\times(2n(r+1)-1)+(3n+2nr-3)\times1]$

+

$\frac{n-1}{2}[(2nr-3r+3n-7)\times3(r+1)+(3r+2)\times(2n-3)(r+1)]$

+

$\frac{n-1}{2}[(2nr-3r+3n-7)\times3(r+1)+(3r+2)\times(2n-3)(r+1)]$

+ $\frac{(n-1)r}{2}[1\times(2n(r+1)-1)+(3n+2nr-3)\times1]$

$=r^2(22n^2-35n+20)+r(\frac{85}{2}n^2-\frac{179}{2}n+50)$

$+(\frac{39}{2}n^2-\frac{101}{2}n+30)$

Corollary 3. $Sz_{ev}(\tilde{F}_n)=\frac{39}{2}n^2-\frac{101}{2}n+30$.

Theorem 6. $Sz_{ev}(I_r(\tilde{W}_n))=r^2(22n^2-16n)$

$+r(\frac{85}{2}n^2-\frac{79}{2}n+2)+(\frac{39}{2}n^2-\frac{47}{2}n-1)$.

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 $v_{n.n+1}=v_{n.1}$, $v_{n+1}=v_1$. In view of the definition of edge-vertex Szeged index, we deduce

$Sz_{ev}(I_r(\tilde{W}_n))=$

$\frac{1}{2}\sum_{i=1}^{r}\sum_{e=uv}(m_{v^i}(vv^i)n_v(vv^i)+m_v(vv^i)n_{v^i}(vv^i))$ +

$\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_i}(vv_i)n_v(vv_i)+m_v(vv_i)n_{v_i}(vv_i))$

+

$\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{e=uv}(m_{v_i^j}(v_iv_i^j)n_{v_i}(v_iv_i^j)+m_{v_i}(v_iv_i^j)n_{v_i^j}(v_iv_i^j))$

+

$\frac{1}{2}\sum_{i=1}^{n}(m_{v_{i,i+1}}(v_iv_{i,i+1})n_{v_i}(v_iv_{i,i+1})+m_{v_i}(v_iv_{i,i+1})n_{v_{i,i+1}}(v_iv_{i,i+1}))$

+

$\frac{1}{2}\sum_{i=1}^{n}(m_{v_{i+1}}(v_{i,i+1}v_{i+1})n_{v_{i,i+1}}(v_{i,i+1}v_{i+1})+m_{v_{i,i+1}}(v_{i,i+1}v_{i+1})n_{v_{i+1}}(v_{i,i+1}v_{i+1}))$

+ $\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}(m_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j)n_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)$

$+m_{v_{i,i+1}}(v_{i,i+1}v_{i,i+1}^j)n_{v_{i,i+1}^j}(v_{i,i+1}v_{i,i+1}^j))$

$=\frac{r}{2}[(3n+2nr+r-1)\times1+1\times(r+2n(r+1)]$

+

$\frac{n}{2}[(3r+2)\times(2n-2)(r+1)+(2nr+3n-2r-5)\times3(r+1)]$

+

$\frac{nr}{2}[1\times((2n+1)(r+1)-1)+(3n+2nr+r-1)\times1]$

+

$$\frac{n}{2}[(2nr-2r+3n-5)\times 3(r+1)+(3r+2)\times(2n-2)(r+1)]$$

$$+\frac{n}{2}[(2nr-2r+3n-5)\times 3(r+1)+(3r+2)\times(2n-2)(r+1)]$$

$$+\frac{nr}{2}[1\times((2n+1)(r+1)-1)+(3n+2nr+r-1)\times 1]$$

$$=r^2(22n^2-16n)+r(\frac{85}{2}n^2-\frac{79}{2}n+2)+(\frac{39}{2}n^2-\frac{47}{2}n-1)$$

Corollary 4. $Sz_{ev}(\tilde{W}_n)=\frac{39}{2}n^2-\frac{47}{2}n-1$.

Theorem 7. $Sz_{ve}(I_r(F_n))=$

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

$$+r^2(2n^3+7n-10)+r(\frac{5}{2}n^3-\frac{13}{2}n^2+\frac{13}{2}n-\frac{55}{2})+(n^3-\frac{9}{2}n^2+15n-19).$$

Proof. Using the definition of vertex-edge Szeged index, we have

$$Sz_{ve}(I_r(F_n))=$$

$$\frac{1}{2}\sum_{i=1}^{r}\sum_{e=uv}(m_{v^i}(vv^i)n_{v^i}(vv^i)+m_v(vv^i)n_v(vv^i))+\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_i}(vv_i)n_{v_i}(vv_i)+m_v(vv_i)n_v(vv_i))$$

$$+\frac{1}{2}\sum_{i=1}^{n-1}\sum_{e=uv}(m_{v_{i+1}}(v_iv_{i+1})n_{v_{i+1}}(v_iv_{i+1})+m_{v_i}(v_iv_{i+1})n_{v_i}(v_iv_{i+1}))$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{e=uv}(m_{v_i^j}(v_iv_i^j)n_{v_i^j}(v_iv_i^j)+m_{v_i}(v_iv_i^j)n_{v_i}(v_iv_i^j))$$

$$=\frac{r}{2}[1\times 1+(2n+r+nr-2)\times(r+n(r+1))]$$

$$+\frac{1}{2}(2[(r+2)\times(r+1)+(2n+nr-2r-4)\times(n-1)(r+1)]$$

$$+(n-2)[(r+2)\times(r+1)+(2n+nr-2r-5)\times(n-2)(r+1)])$$

$$+\frac{1}{2}(2[(2r+3)\times 2(r+1)+(r+1)\times(r+1)]$$

$$+2[(2r+3)\times 2(r+1)+(2r+2)\times 2(r+1)]$$

$$+(n-5)[(2r+3)\times 2(r+1)+(2r+3)\times 2(r+1)])$$

$$+\frac{nr}{2}[1\times 1+(2n+r+nr-2)\times(r+n(r+1))]$$

$$=r^3(\frac{1}{2}n^3+\frac{3}{2}n^2+\frac{3}{2}n+\frac{1}{2})+r^2(2n^3+7n-10)$$

$$+r(\frac{5}{2}n^3-\frac{13}{2}n^2+\frac{13}{2}n-\frac{55}{2})$$

$$+(n^3-\frac{9}{2}n^2+15n-19).$$

Corollary 5. $Sz_{ve}(F_n)=n^3-\frac{9}{2}n^2+15n-19$.

Theorem 8. $Sz_{ve}(I_r(W_n))=$

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

$$+r^2(3n^3+\frac{1}{2}n^2+7n-\frac{1}{2})+r(\frac{5}{2}n^3-6n^2+\frac{35}{2}n)+(n^3-\frac{9}{2}n^2+12n).$$

Proof. In view of the definition of vertex-edge Szeged index, we infer

$$Sz_{ve}(I_r(W_n))=$$

$$\frac{1}{2}\sum_{i=1}^{r}\sum_{e=uv}(m_{v^i}(vv^i)n_{v^i}(vv^i)+m_v(vv^i)n_v(vv^i))$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_i}(vv_i)n_{v_i}(vv_i)+m_v(vv_i)n_v(vv_i))$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_{i+1}}(v_iv_{i+1})n_{v_{i+1}}(v_iv_{i+1})+m_{v_i}(v_iv_{i+1})n_{v_i}(v_iv_{i+1}))$$

$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{e=uv}(m_{v_i^j}(v_iv_i^j)n_{v_i^j}(v_iv_i^j)+m_{v_i}(v_iv_i^j)n_{v_i}(v_iv_i^j))$$

$$=\frac{r}{2}[1\times 1+(2n+r+nr-1)\times(r+n(r+1))]$$

$$+\frac{n}{2}[(r+2)\times(r+1)+(2n+nr-2r-5)\times(n-2)(r+1)]+\frac{n}{2}[(2r+3)\times 2(1+r)+(2r+3)\times 2(1+r)]$$

$$+\frac{nr}{2}[1\times 1+(2n+r+nr-1)\times(r+n(r+1))]$$

$$=r^3(\frac{1}{2}n^3+\frac{3}{2}n^2+\frac{3}{2}n+\frac{1}{2})+r^2(3n^3+\frac{1}{2}n^2+7n-\frac{1}{2})$$

$$+r(\frac{5}{2}n^3-6n^2+\frac{35}{2}n)+(n^3-\frac{9}{2}n^2+12n)$$

Corollary 6. $Sz_{ve}(W_n)=n^3-\frac{9}{2}n^2+12n$.

Theorem 9. $Sz_{ve}(I_r(\tilde{F}_n))=$

$$r^3(4n^3)+r^2(16n^3-30n^2+43n-28)$$
$$+r(21n^3-\frac{143}{2}n^2+117n-\frac{139}{2})+(9n^3-\frac{81}{2}n^2+\frac{141}{2}n-42).$$

Proof. By virtue of the definition of vertex-edge Szeged index, we yield

$$Sz_{ve}(I_r(\tilde{F}_n))=$$
$$\frac{1}{2}\sum_{i=1}^{r}\sum_{e=uv}(m_{v^i}(vv^i)n_{v^i}(vv^i)+m_v(vv^i)n_v(vv^i))+$$
$$\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_i}(vv_i)n_{v_i}(vv_i)+m_v(vv_i)n_v(vv_i))$$
$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{e=uv}(m_{v_i^j}(v_iv_i^j)n_{v_i^j}(v_iv_i^j)+m_{v_i}(v_iv_i^j)n_{v_i}(v_iv_i^j))$$
$$+\frac{1}{2}\sum_{i=1}^{n-1}(m_{v_{i,i+1}}(v_iv_{i,i+1})n_{v_{i,i+1}}(v_iv_{i,i+1})+m_{v_i}(v_iv_{i,i+1})n_{v_i}(v_iv_{i,i+1}))$$
$$+\frac{1}{2}\sum_{i=1}^{n-1}(m_{v_{i+1}}(v_{i,i+1}v_{i+1})n_{v_{i+1}}(v_{i,i+1}v_{i+1})+m_{v_{i,i+1}}(v_{i,i+1}v_{i+1})n_{v_{i,i+1}}(v_{i,i+1}v_{i+1}))$$
$$+\frac{1}{2}\sum_{i=1}^{n-1}\sum_{j=1}^{r}(m_{v^j_{i,i+1}}(v_{i,i+1}v^j_{i,i+1})n_{v^j_{i,i+1}}(v_{i,i+1}v^j_{i,i+1})$$
$$+m_{v_{i,i+1}}(v_{i,i+1}v^j_{i,i+1})n_{v_{i,i+1}}(v_{i,i+1}v^j_{i,i+1}))$$
$$=\frac{r}{2}[1\times1+(3n+2nr-3)\times(r+(r+1)(2n-1)]$$
$$+\frac{1}{2}(2[(2r+1)\times2(r+1)+(2nr+3n-2r-5)\times(2n-2)(r+1)]$$
$$+(n-2)[(3r+2)\times3(r+1)+(2nr+3n-3r-7)\times(2n-3)(r+1)])$$
$$+\frac{nr}{2}[1\times1+(3n+2nr-3)\times(2n(r+1)-1)]$$
$$+\frac{n-1}{2}[(2nr-3r+3n-7)\times(2n-3)(r+1)+(3r+2)\times3(r+1)]$$
$$+\frac{n-1}{2}[(2nr-3r+3n-7)\times(2n-3)(r+1)+(3r+2)\times3(r+1)]$$
$$+\frac{(n-1)r}{2}[(3n+2nr-3)\times(2n(r+1)-1)+1\times1]$$
$$=r^3(4n^3)+r^2(16n^3-30n^2+43n-28)$$
$$+r(21n^3-\frac{143}{2}n^2+117n-\frac{139}{2})+(9n^3-\frac{81}{2}n^2+\frac{141}{2}n-42)$$

Corollary 7. $Sz_{ve}(\tilde{F}_n)=9n^3-\frac{81}{2}n^2+\frac{141}{2}n-42$.

Theorem 10. $Sz_{ve}(I_r(\tilde{W}_n))=$

$$r^3(n^3+\frac{5}{2}n^2+2n+\frac{1}{2})$$
$$+r^2(\frac{19}{2}n^3-\frac{17}{2}n^2-19n-\frac{1}{2})+r(18n^3-34n^2+\frac{85}{2}n)$$
$$+(9n^3-24n^2+24n).$$

Proof. In view of the definition of vertex-edge Szeged index, we deduce

$$Sz_{ve}(I_r(\tilde{W}_n))=$$
$$\frac{1}{2}\sum_{i=1}^{r}\sum_{e=uv}(m_{v^i}(vv^i)n_{v^i}(vv^i)+m_v(vv^i)n_v(vv^i))+$$
$$\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_i}(vv_i)n_{v_i}(vv_i)+m_v(vv_i)n_v(vv_i))$$
$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{e=uv}(m_{v_i^j}(v_iv_i^j)n_{v_i^j}(v_iv_i^j)+m_{v_i}(v_iv_i^j)n_{v_i}(v_iv_i^j))$$
$$+\frac{1}{2}\sum_{i=1}^{n}(m_{v_{i,i+1}}(v_iv_{i,i+1})n_{v_{i,i+1}}(v_iv_{i,i+1})+m_{v_i}(v_iv_{i,i+1})n_{v_i}(v_iv_{i,i+1}))$$
$$+\frac{1}{2}\sum_{i=1}^{n}(m_{v_{i+1}}(v_{i,i+1}v_{i+1})n_{v_{i+1}}(v_{i,i+1}v_{i+1})+m_{v_{i,i+1}}(v_{i,i+1}v_{i+1})n_{v_{i,i+1}}(v_{i,i+1}v_{i+1}))$$
$$+\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}(m_{v^j_{i,i+1}}(v_{i,i+1}v^j_{i,i+1})n_{v^j_{i,i+1}}(v_{i,i+1}v^j_{i,i+1})$$
$$+m_{v_{i,i+1}}(v_{i,i+1}v^j_{i,i+1})n_{v_{i,i+1}}(v_{i,i+1}v^j_{i,i+1}))$$
$$=\frac{r}{2}[1\times1+(3n+2nr+r-1)\times(r+2n(r+1)]$$
$$+$$

$$\frac{n}{2}[(3r+2)\times 3(r+1)+(2nr+3n-2r-5)\times(2n-2)(r+1)]$$

+

$$\frac{nr}{2}[1\times 1+(3n+2nr+r-1)\times((2n+1)(r+1)-1)]$$

+

$$\frac{n}{2}[(2nr-2r+3n-5)\times(2n-2)(r+1)+(3r+2)\times 3(r+1)]$$

+

$$\frac{n}{2}[(2nr-2r+3n-5)\times(2n-2)(r+1)+(3r+2)\times 3(r+1)]$$

+

$$\frac{nr}{2}[1\times 1+(3n+2nr+r-1)\times((2n+1)(r+1)-1)]$$

=

$$r^3(n^3+\frac{5}{2}n^2+2n+\frac{1}{2})+r^2(\frac{19}{2}n^3-\frac{17}{2}n^2-19n-\frac{1}{2})$$

$$+r(18n^3-34n^2+\frac{85}{2}n)+(9n^3-24n^2+24n).$$

Corollary 8. $Sz_{ve}(\tilde{W}_n) = 9n^3-24n^2+24n$.

III. CONCLUSION AND DISCUSSION

Corollary 7. $Sz_{ve}(\tilde{F}_n) = 9n^3-\frac{81}{2}n^2+\frac{141}{2}n-42$.

Theorem 10. $Sz_{ve}(I_r(\tilde{W}_n)) =$

$$r^3(n^3+\frac{5}{2}n^2+2n+\frac{1}{2})$$

$$+r^2(\frac{19}{2}n^3-\frac{17}{2}n^2-19n-\frac{1}{2})+r(18n^3-34n^2+\frac{85}{2}n)$$

$$+(9n^3-24n^2+24n).$$

Proof. In view of the definition of vertex-edge Szeged index, we deduce

$Sz_{ve}(I_r(\tilde{W}_n)) =$

$$\frac{1}{2}\sum_{i=1}^{r}\sum_{e=uv}(m_{v^i}(vv^i)n_{v^i}(vv^i)+m_v(vv^i)n_v(vv^i)) +$$

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{e=uv}(m_{v_i}(vv_i)n_{v_i}(vv_i)+m_v(vv_i)n_v(vv_i))$$

+

$$\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{r}\sum_{e=uv}(m_{v_i^j}(v_iv_i^j)n_{v_i^j}(v_iv_i^j)+m_{v_i}(v_iv_i^j)n_{v_i}(v_iv_i^j))$$

+

$$\frac{1}{2}\sum_{i=1}^{n}(m_{v_{i,i+1}}(v_iv_{i,i+1})n_{v_{i,i+1}}(v_iv_{i,i+1})+m_{v_i}(v_iv_{i,i+1})n_{v_i}(v_iv_{i,i+1}))$$

+

$$\frac{1}{2}\sum_{i=1}^{n}(m_{v_{i+1}}(v_{i,i+1}v_{i+1})n_{v_{i+1}}(v_{i,i+1}v_{i+1})+m_{v_{i,i+1}}(v_{i,i+1}v_{i+1})n_{v_{i,i+1}}(v_{i,i+1}v_{i+1}))$$

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

$$+m_{v_{i,i+1}}(v_{i,i+1}v^j_{i,i+1})n_{v_{i,i+1}}(v_{i,i+1}v^j_{i,i+1}))$$

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

+

$$\frac{n}{2}[(3r+2)\times 3(r+1)+(2nr+3n-2r-5)\times(2n-2)(r+1)]$$

+

$$\frac{nr}{2}[1\times 1+(3n+2nr+r-1)\times((2n+1)(r+1)-1)]$$

+

$$\frac{n}{2}[(2nr-2r+3n-5)\times(2n-2)(r+1)+(3r+2)\times 3(r+1)]$$

+

$$\frac{n}{2}[(2nr-2r+3n-5)\times(2n-2)(r+1)+(3r+2)\times 3(r+1)]$$

+

$$\frac{nr}{2}[1\times 1+(3n+2nr+r-1)\times((2n+1)(r+1)-1)]$$

=

$$r^3(n^3+\frac{5}{2}n^2+2n+\frac{1}{2})+r^2(\frac{19}{2}n^3-\frac{17}{2}n^2-19n-\frac{1}{2})$$

$$+r(18n^3-34n^2+\frac{85}{2}n)+(9n^3-24n^2+24n)$$

Corollary 8. $Sz_{ve}(\tilde{W}_n) = 9n^3-24n^2+24n$.

3. DISCUSSION

Theorems 1 and 2 establish that the graph with n vertices, connectivity k, and minimum Hyper-Wiener index is same in the case of vertex and edge-connectivity. One may wonder whether Theorem 1 implies Theorem 2, or vice versa. It appears (at least within the present considerations) that the proofs of these two theorems are independent.

As already mentioned, the 1- and 2-connected graphs with maximum Hyper-Wiener indices are known. The natural question at this point is to ask for k-connected ($k \geq 2$), n-vertex graphs having maximum Hyper-Wiener index. This problem seems to be much more difficult, and, at this moment, we cannot offer any solution of it, not even for the case *k*=3.

Another related question is whether *n*-vertex, *k*-vertex connected and *n*-vertex, *k*-edge connected graphs with maximum Hyper-Wiener index differ at all, and if yes, for which values of *k* and *n*.

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REFERENCES

[1] L. Yan, Y. Li, W. Gao, and J. Li, "On the extremal hyper-wiener index of graphs", Journal of Chemical and Pharmaceutical Research, vol. 6, no. 3, 2014, pp. 477-481.

[2] L. Yan, Y. Li, W. Gao, and J. Li, "PI index for some special graphs", Journal of Chemical and Pharmaceutical Research, vol. 5, no. 11, 2013, pp. 260-264.

[3] W. Gao and L. Shi, "Wiener index of gear fan graph and gear wheel graph", Asian Journal of Chemistry, vol. 26, no. 11, 2014, pp. 3397-3400.

[4] Y. Gao, L. Liang, and W. Gao, "Eccentric connectivity index of some special molecular graphs and their *r*-corona graphs", International Journal of Chemical and Process Engineering Research, vol. 1, no.5, 2014, pp. 43-50.

[5] Y. Gao, L. Liang, and W. Gao, "Randic index and edge eccentric connectivity index of certain special molecular graphs", International Journal of Chemistry and Materials Research, vol. 2, no.8, 2014, pp. 81-87.

[6] W. Xi and W. Gao, "Geometric-arithmetic index and Zagreb indices of certain special molecular graphs", Journal of Advances in Chemistry, vol. 10, no.2, 2014, pp. 2254-2261

[7] M. Alaeiyan and J. Asadpour, "The vertex-edge Szeged index of bridge graphs", World Applied Sciences Journal, vol. 14, no. 8, 2011, pp. 1254-1257.