Revised Szeged Index and Revised Edge Szeged Index of Certain Special Molecular Graphs

Yun Gao¹, Wei Gao^{2*}, Li Liang²

- ¹ Department of Editorial, Yunnan Normal University, Kunming 650092, China.
- ² School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China.
- * Corresponding author. Tel.:+86 13756543457; email: gaowei@ynnu.edu.cn Manuscript submitted September 26, 2014; accepted November 24, 2014. doi: 10.17706/ijapm.2014.4.6.417-425

Abstract: In theoretical chemistry, the revised Szeged index and revised Szeged edge index were introduced to measure the stability of alkanes and the strain energy of cycloalkanes. In this paper, by virtue of mathematical derivation, we determine the revised Szeged index and revised edge Szeged index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs. These molecular structures are widely used in biology, medical science and pharmaceutical fields. At last, the normalized revised Szeged indexes of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their r-corona molecular graphs are given.

Key words: Chemical graph theory, revised Szeged index, revised edge Szeged index, fan molecular graph, wheel molecular graph, gear fan molecular graph, Gear wheel molecular graph, r-corona molecular graph.

1. Introduction

Wiener index, PI index, revised Szeged index and revised 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] for more detail). Let P_n and C_n be path and cycle with n vertices. The molecular graph $F_n = \{v\} \lor P_n$ is called a fan molecular graph and the molecular graph $W_n = \{v\} \lor C_n$ 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 .

Let e=uv be an edge of the molecular graph G. The number of vertices of G whose 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 v. Let n(e) be the number of vertices equidistant from both ends of $uv \in E(G)$, The revised Szeged index is defined as

$$Sz^*(G) = \sum_{e=uv} (n_u(e) + \frac{n(e)}{2})(n_v(e) + \frac{n(e)}{2}).$$

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. Let m(e) be the number of edges equidistant from both ends of $uv \in E(G)$. The revised edge Szeged index of G is defined as

$$Sz_e^*(G) = \sum_{e=uv} (m_u(e) + \frac{m(e)}{2})(m_v(e) + \frac{m(e)}{2}).$$

Xing and Zhou [4] determined the *n*-vertex unicyclic graphs with the smallest, the second-smallest and the third-smallest revised Szeged index. Chen *et al.* [5] studied the differences between the revised Szeged index and the Wiener index. Dong *et al.* [6] considered the revised edge Szeged index of molecular graphs. Faghani and Ashrafi [7] presented new formula for computing molecular descriptor.

In this paper, we present the revised Szeged index and revised edge Szeged index of $I_r(F_n)$, $I_r(W_n)$, $I_r(\tilde{F}_n)$ and $I_r(\tilde{W}_n)$

2. Revised Szeged Index

Theorem 1.
$$Sz^*(I_r(F_n)) = r^2(\frac{n^3}{4} + \frac{15}{4}n^2 - \frac{1}{4}n + \frac{11}{4}) + r(\frac{n^3}{2} + \frac{13}{2}n^2 - \frac{7}{2}n + \frac{7}{2}) + (\frac{n^3}{4} + \frac{1}{4}n^2 - \frac{9}{4}n + \frac{7}{4}).$$

Proof. Let $P_n = v_1 v_2 ... v_n$ 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^r . Using the definition of revised Szeged index, we have

$$\begin{split} Sz^*(I_r(F_n)) &= \sum_{i=1}^r \sum_{e=uv} (n_v(vv^i) + \frac{n(vv^i)}{2})(n_{v^i}(vv^i) + \frac{n(vv^i)}{2}) + \\ &\sum_{i=1}^n \sum_{e=uv} (n_v(vv_i) + \frac{n(vv_i)}{2})(n_{v_i}(vv_i) + \frac{n(vv_i)}{2}) + \sum_{i=1}^{n-1} \sum_{e=uv} (n_v(v_iv_{i+1}) + \frac{n(v_iv_{i+1})}{2})(n_{v_i}(v_iv_{i+1}) + \frac{n(v_iv_{i+1})}{2}) \\ &+ \sum_{i=1}^n \sum_{j=1}^r \sum_{e=uv} (n_{v_i}(v_iv_i^j) + \frac{n(v_iv_i^j)}{2})(n_{v_i^j}(v_iv_i^j) + \frac{n(v_iv_i^j)}{2}) \\ &= r(r + n(r+1)) + (2(r+1 + \frac{r+1}{2})[(n-1)(r+1) + \frac{r+1}{2}] + (n-2)2(r+1)[(n-1)(r+1)]) + \\ &2(r+1 + \frac{(n-2)(r+1)}{2})[2(r+1) + \frac{(n-2)(r+1)}{2}] + (n-3)(2(r+1) + \frac{(n-3)(r+1)}{2})(2(r+1) + \frac{(n-3)(r+1)}{2}) + \\ &\qquad \qquad nr(r+n(r+1)) \\ &= r^2(\frac{n^3}{4} + \frac{15}{4}n^2 - \frac{1}{4}n + \frac{11}{4}) + r(\frac{n^3}{2} + \frac{13}{2}n^2 - \frac{7}{2}n + \frac{7}{2}) + (\frac{n^3}{4} + \frac{1}{4}n^2 - \frac{9}{4}n + \frac{7}{4}) \,. \end{split}$$

Corollary 1.
$$Sz^*(F_n) = \frac{n^3}{4} + \frac{1}{4}n^2 - \frac{9}{4}n + \frac{7}{4}$$
.

Theorem 2.
$$Sz^*(I_r(W_n)) = r^2(\frac{n^3}{4} + \frac{7}{2}n^2 + \frac{1}{4}n + 1) + r(\frac{n^3}{2} + 6n^2 - \frac{5}{2}n) + (\frac{n^3}{4} + \frac{5}{2}n^2 - \frac{7}{4}n)$$
.

Proof. Let $C_n = v_1 v_2 ... v_n$ 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 $v_n v_{n+1} = v_n v_1$. In view of the definition of revised Szeged index, we infer

$$Sz^{*}(I_{r}(W_{n})) = \sum_{i=1}^{r} \sum_{e=uv} (n_{v}(vv^{i}) + \frac{n(vv^{i})}{2})(n_{v^{i}}(vv^{i}) + \frac{n(vv^{i})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (n_{v}(vv_{i}) + \frac{n(vv_{i})}{2})(n_{v_{i}}(vv_{i}) + \frac{n(vv_{i})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (n_{v_{i}}(v_{i}v_{i+1}) + \frac{n(v_{i}v_{i+1})}{2})(n_{v_{i+1}}(v_{i}v_{i+1}) + \frac{n(v_{i}v_{i+1})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} \sum_{e=uv} (n_{v_{i}}(v_{i}v_{i}^{j}) + \frac{n(v_{i}v_{i}^{j})}{2})(n_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{n(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} \sum_{e=uv} (n_{v_{i}}(v_{i}v_{i}^{j}) + \frac{n(v_{i}v_{i}^{j})}{2})(n_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{n(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} \sum_{e=uv} (n_{v_{i}}(v_{i}v_{i}^{j}) + \frac{n(v_{i}v_{i}^{j})}{2})(n_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{n(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (n_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{n(v_{i}v_{i}^{j})}{2})(n_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{n(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (n_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{n(v_{i}^{j}v_{$$

Corollary 2. $Sz^*(W_n) = \frac{n^3}{4} + \frac{5}{2}n^2 - \frac{7}{4}n$.

Theorem 3.
$$Sz^*(I_r(\tilde{F}_n)) = r^2(22n^2 - 43n + 28) + r(40n^2 - 88n + 56) + (18n^2 - 43n + 28)$$
.

Proof. Let $P_n = v_1 v_2 ... v_n$ 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_i^1 be a vertex in v_i^2 , and the v_i^2 hanging vertices of v_i^2 , ..., v_i^2 , ..., v_i^2 .

By virtue of the definition of revised Szeged index, we yield

$$\begin{split} Sz^*(I_r(\tilde{F}_n)) &= \sum_{i=1}^r \sum_{e=uv} (n_v(vv^i) + \frac{n(vv^i)}{2}) (n_{v^i}(vv^i) + \frac{n(vv^i)}{2}) + \\ &\sum_{i=1}^n \sum_{e=uv} (n_v(vv_i) + \frac{n(vv_i)}{2}) (n_{v_i}(vv_i) + \frac{n(vv_i)}{2}) + \sum_{i=1}^n \sum_{j=1}^r \sum_{e=uv} (n_{v_i}(v_iv_i^j) + \frac{n(v_iv_i^j)}{2}) (n_{v_i^j}(v_iv_i^j) + \frac{n(v_iv_i^j)}{2}) \\ &\quad + \sum_{i=1}^{n-1} (n_{v_i}(v_iv_{i,i+1}) + \frac{n(v_iv_{i,i+1})}{2}) (n_{v_{i,i+1}}(v_iv_{i,i+1}) + \frac{n(v_iv_{i,i+1})}{2}) \\ &\quad + \sum_{i=1}^{n-1} (n_{v_{i,i+1}}(v_{i,i+1}v_{i+1}) + \frac{n(v_{i,i+1}v_{i+1})}{2}) (n_{v_{i+1}}(v_{i,i+1}v_{i+1}) + \frac{n(v_{i,i+1}v_{i+1})}{2}) \\ &\quad + \sum_{i=1}^{n-1} \sum_{j=1}^r (n_{v_{i,i+1}}(v_{i,i+1}v_{i,j+1}^j) + \frac{n(v_{i,i+1}v_{i,j+1}^j)}{2}) (n_{v_{i,i+1}}(v_{i,i+1}v_{i,j+1}^j) + \frac{n(v_{i,i+1}v_{i,j+1}^j)}{2}) \\ &\quad = r(r + (r+1)(2n-1)) + 2(2n-2)(r+1)2(r+1) + (n-2)(2n-3)(r+1)3(r+1) \\ &\quad + nr(r + (r+1)(2n-1)) + (n-1)(2n-3)(r+1)3(r+1) + (n-1)(2n-3)(r+1)3(r+1) \\ &\quad + (n-1)r(r + (r+1)(2n-1)) = r^2(22n^2 - 43n + 28) + r(40n^2 - 88n + 56) + (18n^2 - 43n + 28) \,. \end{split}$$

Corollary 3. $Sz^*(\tilde{F}_n) = 18n^2 - 43n + 28$.

Theorem 4.
$$Sz^*(I_r(\tilde{W}_n)) = r^2(22n^2 - 14n + 1) + r(40n^2 - 34n) + (18n^2 - 18n)$$
.

Proof. Let $C_n = v_1 v_2 ... v_n$ 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^1_i , v^2_i , ..., v^r_i be the r hanging vertices of $v_i (1 \le i \le n)$. Let $v_{n,n+1} = v_{1,n}$ and $v^1_{i,i+1}$, $v^2_{i,i+1}$, ..., $v^r_{i,i+1}$ be the r hanging vertices of $v_{i,i+1}$ ($1 \le i \le n$). Let $v_{n,n+1} = v_{n,1}$, $v_{n+1} = v_{n,1}$. In view of the definition of revised Szeged index, we deduce

$$\begin{split} Sz^*(I_r(\tilde{W_n})) &= \sum_{i=1}^r \sum_{e=uv} (n_v(vv^i) + \frac{n(vv^i)}{2}) (n_{v^i}(vv^i) + \frac{n(vv^i)}{2}) + \\ \sum_{i=1}^n \sum_{e=uv} (n_v(vv_i) + \frac{n(vv_i)}{2}) (n_{v_i}(vv_i) + \frac{n(vv_i)}{2}) + \sum_{i=1}^r \sum_{j=1}^r \sum_{e=uv} (n_{v_i}(v_iv_i^j) + \frac{n(v_iv_i^j)}{2}) (n_{v_i^j}(v_iv_i^j) + \frac{n(v_iv_i^j)}{2}) \\ &+ \sum_{i=1}^n (n_{v_i}(v_iv_{i,i+1}) + \frac{n(v_iv_{i,i+1})}{2}) (n_{v_{i,i+1}}(v_iv_{i,i+1}) + \frac{n(v_iv_{i,i+1})}{2}) \\ &+ \sum_{i=1}^n (n_{v_{i,i+1}}(v_{i,i+1}v_{i+1}) + \frac{n(v_{i,i+1}v_{i+1})}{2}) (n_{v_{i+1}}(v_{i,i+1}v_{i+1}) + \frac{n(v_{i,i+1}v_{i+1})}{2}) \\ &+ \sum_{i=1}^n \sum_{j=1}^r (n_{v_{i,i+1}}(v_{i,i+1}v_{i,j+1}^j) + \frac{n(v_{i,i+1}v_{i,j+1}^j)}{2}) (n_{v_{i,i+1}}^j(v_{i,i+1}v_{i,j+1}^j) + \frac{n(v_{i,i+1}v_{i,j+1}^j)}{2}) \\ &= r(r+2n(r+1)) + n(2n-2)(r+1)3(r+1) + nr(r+2n(r+1)) + n(2n-2)(r+1)3(r+1) \\ &+ n(2n-2)(r+1)3(r+1) + nr(r+2n(r+1)) \\ &= r^2(22n^2 - 14n + 1) + r(40n^2 - 34n) + (18n^2 - 18n) \, . \end{split}$$

Corollary 4. $Sz^*(\tilde{W_n}) = 18n^2 - 18n$.

3. Revised Edge Szeged Index

Theorem 5.
$$Sz_{\epsilon}^{*}(I_{r}(F_{n})) = r^{2}(\frac{n^{3}}{4} + \frac{7}{2}n^{2} + \frac{3}{4}n + 3) + r(n^{3} + \frac{19}{2}n^{2} - \frac{27}{2}n + \frac{9}{2}) + (n^{3} + 5n^{2} - \frac{63}{4}n + 13).$$

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

$$Sz_{e}^{*}(I_{r}(F_{n})) = \sum_{i=1}^{r} \sum_{e=uv} (m_{v}(vv^{i}) + \frac{m(vv^{i})}{2})(m_{v_{i}}(vv^{i}) + \frac{m(vv^{i})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (m_{v}(vv_{i}) + \frac{m(vv_{i})}{2})(m_{v_{i}}(vv_{i}) + \frac{m(vv_{i})}{2}) + \sum_{i=1}^{n-1} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i+1}) + \frac{m(v_{i}v_{i+1})}{2})(m_{v_{i+1}}(v_{i}v_{i+1}) + \frac{m(v_{i}v_{i+1})}{2}) + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2})(m_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2})(m_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2})(m_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2})(m_{v_{i}^{j}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}) + \frac{m(v_{i}v_{i})}{2})(m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i})}{2}) + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}) + \frac{m(v_{i}v_{i})}{2})(m_{v_{i}}(v_{i}v_{i}) + \frac{m(v_{i}v_{i})}{2}) + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}) + \frac{m(v_{i}v_{i})}{2})(m_{v_{i}}(v_{i}v_{i}) + \frac{m(v_{i}v_{i})}{2}) + \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}) + \frac{m(v_{i}v_{i})}{2})(m_{v_{i}}(v_{i}v_{i}) + \frac{m(v_{i}v_{i})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i$$

$$(n-4)(2r+3+\frac{nr+2n-3r-7}{2})(2r+3+\frac{nr+2n-3r-7}{2}))+nr(2n+r+nr-2)$$

$$=r^2(\frac{n^3}{4}+\frac{7}{2}n^2+\frac{3}{4}n+3)+r(n^3+\frac{19}{2}n^2-\frac{27}{2}n+\frac{9}{2})+(n^3+5n^2-\frac{63}{4}n+13)\,.$$

Corollary 5. $Sz_e^*(F_n) = n^3 + 5n^2 - \frac{63}{4}n + 13$

Theorem 6.
$$Sz_{\epsilon}^{*}(I_{r}(W_{n})) = r^{2}(\frac{n^{3}}{4} + \frac{7}{2}n^{2} + \frac{1}{4}n + 1) + r(n^{3} + \frac{21}{2}n^{2} - \frac{19}{2}n - 1) + (n^{3} + 7n^{2} - \frac{49}{4}n)$$
.

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

$$Sz_{e}^{*}(I_{r}(W_{n})) = \sum_{i=1}^{r} \sum_{e=uv} (m_{v}(vv^{i}) + \frac{m(vv^{i})}{2})(m_{v^{i}}(vv^{i}) + \frac{m(vv^{i})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (m_{v}(vv_{i}) + \frac{m(vv_{i})}{2})(m_{v_{i}}(vv_{i}) + \frac{m(vv_{i})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i+1}) + \frac{m(v_{i}v_{i+1})}{2})(m_{v_{i+1}}(v_{i}v_{i+1}) + \frac{m(v_{i}v_{i+1})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2})(m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2})(m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}^{j}) +$$

Corollary6. $Sz_e^*(W_n) = n^3 + 7n^2 - \frac{49}{4}n$.

Theorem 7.
$$Sz_{\epsilon}^*(I_r(\tilde{F}_n)) = r^2(20n^2 - 31n + 16) + r(44n^2 - \frac{221}{2}n + \frac{147}{2}) + (21n^2 - 58n + \frac{167}{4})$$
.

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

$$\begin{split} Sz_{_{e}}^{*}(I_{_{r}}(\tilde{F}_{_{n}})) &= \sum_{i=1}^{r} \sum_{e=uv} (m_{_{v}}(vv^{i}) + \frac{m(vv^{i})}{2})(m_{_{v^{i}}}(vv^{i}) + \frac{m(vv^{i})}{2}) + \sum_{i=1}^{n} \sum_{e=uv} (m_{_{v}}(vv_{_{i}}) + \frac{m(vv_{_{i}})}{2})(m_{_{v_{_{i}}}}(v_{_{i}}v^{j}_{_{i}}) + \frac{m(v_{_{i}}v^{j}_{_{i}})}{2}) \\ &+ \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{_{v_{_{i}}}}(v_{_{i}}v^{j}_{_{i}}) + \frac{m(v_{_{i}}v^{j}_{_{i}})}{2})(m_{_{v_{_{i}}}}(v_{_{i}}v^{j}_{_{i}}) + \frac{m(v_{_{i}}v^{j}_{_{i}})}{2}) \\ &+ \sum_{i=1}^{n-1} (m_{_{v_{_{i},i+1}}}(v_{_{i,i+1}}v_{_{i+1}}) + \frac{m(v_{_{i}}v_{_{i,i+1}}}{2})(m_{_{v_{_{i,i+1}}}}(v_{_{i,i+1}}v_{_{i+1}}) + \frac{m(v_{_{i}}v_{_{i,i+1}}}{2}) \\ &+ \sum_{i=1}^{n-1} \sum_{j=1}^{r} (m_{_{v_{_{i,i+1}}}}(v_{_{i,i+1}}v^{j}_{_{i,j+1}}) + \frac{m(v_{_{i,i+1}}v^{j}_{_{i,j+1}}}{2})(m_{_{v_{_{i,i+1}}}}(v_{_{i,i+1}}v^{j}_{_{i,j+1}}) + \frac{m(v_{_{i,i+1}}v^{j}_{_{i,j+1}})}{2}) \\ &+ \sum_{i=1}^{n-1} \sum_{j=1}^{r} (m_{_{v_{_{i,i+1}}}}(v_{_{i,i+1}}v^{j}_{_{i,j+1}}) + \frac{m(v_{_{i,i+1}}v^{j}_{_{i,j+1}})}{2})(m_{_{v_{_{i,i+1}}}}(v_{_{i,i+1}}v^{j}_{_{i,j+1}}) + \frac{m(v_{_{i,i+1}}v^{j}_{_{i,j+1}})}{2}) \\ &= r(3n + 2nr - 3) + (2(2r + 2)(2nr + 3n - 2r - 4) + (n - 2)(3r + 2 + \frac{3}{2})(2nr + 3n - 3r - 7 + \frac{3}{2})) + nr(3n + 2nr - 3) + \frac{3}{2}(nr + 2n$$

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

$$=r^2(20n^2-31n+16)+r(44n^2-\frac{221}{2}n+\frac{147}{2})+(21n^2-58n+\frac{167}{4}).$$

Corollary 7.
$$Sz_{e}^{*}(\tilde{F}_{n}) = 21n^{2} - 58n + \frac{167}{4}$$
.

Theorem 8.
$$Sz_{\epsilon}^*(I_r(\tilde{W}_n)) = r^2(22n^2 - 14n + 1) + r(54n^2 - \frac{103}{2}n - 1) + (\frac{63}{2}n^2 - \frac{105}{2}n)$$
.

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

$$\begin{split} Sz_{\epsilon}^{*}(I_{r}(\tilde{W}_{n})) &= \sum_{i=1}^{r} \sum_{e=uv} (m_{v}(vv^{i}) + \frac{m(vv^{i})}{2})(m_{v^{i}}(vv^{i}) + \frac{m(vv^{i})}{2}) + \\ & \sum_{i=1}^{n} \sum_{e=uv} (m_{v}(vv_{i}) + \frac{m(vv_{i})}{2})(m_{v_{i}}(vv_{i}) + \frac{m(vv_{i})}{2}) \\ &+ \sum_{i=1}^{n} \sum_{j=1}^{r} \sum_{e=uv} (m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2})(m_{v_{i}}(v_{i}v_{i}^{j}) + \frac{m(v_{i}v_{i}^{j})}{2}) \\ &+ \sum_{i=1}^{n} (m_{v_{i}}(v_{i}v_{i,i+1}) + \frac{m(v_{i}v_{i,i+1})}{2})(m_{v_{i,i+1}}(v_{i,v_{i+1}}) + \frac{m(v_{i}v_{i,i+1})}{2}) \\ &+ \sum_{i=1}^{n} (m_{v_{i,i+1}}(v_{i,i+1}v_{i+1}) + \frac{m(v_{i,i+1}v_{i+1})}{2})(m_{v_{i,i+1}}(v_{i,i+1}v_{i+1}) + \frac{m(v_{i,i+1}v_{i+1})}{2}) \\ &+ \sum_{i=1}^{n} \sum_{j=1}^{r} (m_{v_{i,i+1}}(v_{i,i+1}v_{j}^{j}) + \frac{m(v_{i,i+1}v_{j}^{j})}{2})(m_{v_{i,i+1}}(v_{i,i+1}v_{j}^{j}) + \frac{m(v_{i,i+1}v_{j}^{j})}{2}) \\ &= r(2nr + 3n + r - 1) + n(3r + 2 + \frac{3}{2})(2nr + 3n - 2r - 5 + \frac{3}{2}) + nr(2nr + 3n + r - 1) + \\ n(3r + 2 + \frac{3}{2})(2nr + 3n - 2r - 5 + \frac{3}{2}) + n(3r + 2 + \frac{3}{2})(2nr + 3n - 2r - 5 + \frac{3}{2}) + nr(2nr + 3n + r - 1) \\ &= r^{2}(22n^{2} - 14n + 1) + r(54n^{2} - \frac{103}{2}n - 1) + (\frac{63}{2}n^{2} - \frac{105}{2}n) \,. \end{split}$$

Corollary 8. $Sz_{e}^{*}(\tilde{W}_{n}) = \frac{63}{2}n^{2} - \frac{105}{2}n$.

4. Normalized Revised Szeged Index

Let m be the edge number of molecular graph G. An Annal Hansen [8] defined the normalized revised Szeged index by dividing $Szs^*(G)$ by m and then taking the square root, i.e.,

$$Szs^*(G) = \sqrt{\frac{Sz^*(G)}{m}}$$
.

Using the conclusions raised in Section 2, we infer the following results concern normalized revised Szeged index.

Theorem 9.

$$Szs^{*}(I_{r}(F_{n})) = \sqrt{\frac{r^{2}(\frac{n^{3}}{4} + \frac{15}{4}n^{2} - \frac{1}{4}n + \frac{11}{4}) + r(\frac{n^{3}}{2} + \frac{13}{2}n^{2} - \frac{7}{2}n + \frac{7}{2}) + (\frac{n^{3}}{4} + \frac{1}{4}n^{2} - \frac{9}{4}n + \frac{7}{4})}{nr + 2n + r - 1}}.$$

Corollary 9.

$$Szs^*(F_n) = \sqrt{\frac{n^3}{4} + \frac{1}{4}n^2 - \frac{9}{4}n + \frac{7}{4}}$$

Theorem 10.

$$Szs^{*}(I_{r}(W_{n})) = \sqrt{\frac{r^{2}(\frac{n^{3}}{4} + \frac{7}{2}n^{2} + \frac{1}{4}n + 1) + r(\frac{n^{3}}{2} + 6n^{2} - \frac{5}{2}n) + (\frac{n^{3}}{4} + \frac{5}{2}n^{2} - \frac{7}{4}n)}{(n+1)r + 2n}}.$$

Corollary 10.

$$Szs^*(W_n) = \sqrt{\frac{n^3 + \frac{5}{2}n^2 - \frac{7}{4}n}{2n}}$$
.

Theorem 11.

$$Szs^{*}(I_{r}(\tilde{F}_{n})) = \sqrt{\frac{r^{2}(22n^{2} - 43n + 28) + r(40n^{2} - 88n + 56) + (18n^{2} - 43n + 28)}{2nr + 3n - 2}}.$$

Corollary 11.

$$Szs^*(\tilde{F}_n) = \sqrt{\frac{18n^2 - 43n + 28}{3n - 2}}$$
.

Theorem 12.

$$Szs^*(I_r(\tilde{W_n})) = \sqrt{\frac{r^2(22n^2 - 14n + 1) + r(40n^2 - 34n) + (18n^2 - 18n)}{(2n + 1)r + 3n}}.$$

Corollary 12.

$$Szs^*(\tilde{W_n}) = \sqrt{\frac{18n^2 - 18n}{3n}}$$
.

5. Conclusion

In this paper, we conduct the revised Szeged index and revised edge Szeged index and third geometric-arithmetic index of fan molecular graph, wheel molecular graph, gear fan molecular graph, gear wheel molecular graph, and their *r*-corona molecular graphs. Furthermore, the normalized revised Szeged indexes of these molecular graphs are manifested. The result achieved in our paper illustrates the promising application prospects for chemical engineering.

Acknowledgements

First, we thank the reviewers for their constructive comments in improving the quality of this paper. This work was supported in part by the National Natural Science Foundation of China (61262071), and the Key Science and Technology Research Project of Education Ministry (210210). We also would like to thank the anonymous referees for providing us with constructive comments and suggestions.

References

- [1] Yan, L., Li, Y., Gao, W., & Li, J. (2014). On the extremal hyper-wiener index of graphs. *Journal of Chemical and Pharmaceutical Research*, *6*(3), 477-481.
- [2] Yan, L., Li, Y., Gao, W., & Li, J. (2013). PI index for some special graphs. *Journal of Chemical and Pharmaceutical Research*, *5*(11), 260-264.
- [3] Gao, W., & Shi, L. (2014). Wiener index of gear fan graph and gear wheel graph. *Asian Journal of Chemistry*, *26*(*11*), 3397-3400.
- [4] Xing, R., & Zhou, B. (2011). On the revised Szeged index. *Discrete Applied Mathematics*, 159, 69-78.
- [5] Chen, L., Li, X., & Liu, M. (2014). The (revised) Szeged index and the Wiener index of a nonbipartite graph. *European Journal of Combinatorics*, *36*, 237-246.
- [6] Dong, H., Zhou, B., & Trinajstic, N. (2011). A novel version of the edge-Szeged index. *Croat. Chem. Acta,* 84(4), 543–545.
- [7] Faghani, M., & Ashrafi, A. R. (2014). Revised and edge revised Szeged indices of graphs. *Ars Mathematica Contemporanea*, *7*, 153–160.
- [8] Aouchiche, M., & Hansen, P. (2012). The normalized revised Szeged index. *MATCH Commun. Math. Comput. Chem.*, 67, 369-381.



Yun Gao was born in Yunnan Province, China, on December 10, 1964. He studied in the Department of Physics of Yunnan Normal University from 1980 to 1984 and got his bachelor degree on physics. And then he worked as an editor and a physics lecturer in the Journal of Yunnan Normal University till now. During this years, he was always engaged in studying the computational physics and other related areas, such as condensed matter physics and computer science. He had published more than 30

scientific papers in home and abroad. Now, as the vice editor in chief of Yunnan Normal University and a researcher, his interests are mainly in computational physics and computing method.



Wei Gao was born in the City of Shaoxing, Zhejiang Province, China on February 13, 1981. He got two bachelor degrees on computer science from Zhejiang Industrial University in 2004 and mathematics education form College of Zhejiang Education in 2006. Then, he enrolled in the Department of Computer Science and Information Technology, Yunnan Normal University, and got his master degree there in 2009. In 2012, he got PhD degree in the Department of Mathematics, Soochow University, China.

Now, he acts as a lecturer in the Department of Information, Yunnan Normal University. As a researcher in computer science and mathematics, his interests are covered two disciplines: graph theory, statistical learning theory, information retrieval, and artificial intelligence.



Li Liang was born in 1965. As a professor of Yunnan Normal University, his interests are in graph theory, statistical learning theory, information retrieval, and artificial intelligence.