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Edge szeged index of certain special molecular graphs

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ABSTRACT

Szeged index and edge Szeged index are introduced to measure the characters of molecular graphs. These properties have potential applications in pharmaceutical field. In this paper, we determine theedgeSzeged 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; Edge Szeged index; Fan molecular graph; Wheel molecular graph; Gear fan moleculargraph; Gear wheel moleculargraph; *r*-corona moleculargraph.

INTRODUCTION

Wiener index,PI indexand Zagreb indicesare 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). LetP_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 $\tilde{W}_n$.

Let $e=uv$ be an edge of the molecular graph G. The number of edges of G whose distance to the vertex u is smaller than thedistance 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. Note that edges equidistant to u and v are not counted. The edgeSzegedindex of G is defined as

$$Sz_e(G) = \sum_{e=uv} m_u(e) m_v(e).$$

Cai and Zhou[4]determined the n-vertex unicyclic graphs with the largest, thesecond largest, the smallest and the second smallest edge Szeged indices. Mahmiani andIranmanesh[5] computed the edge-Szeged index of HAC5C7 nanotube. Chiniforooshan[6] presented the molecular graphs with maximum edge Szeged index. Khalifehet. al.,[7] studied the edge Szeged index of Hamming molecular graphs and C4-nanotubes. Zhan and Qiao[8] determined the edge Szeged index of bridge molecular graph. Gutman and. Ashrafi[9] established the basic properties of edge Szeged index. Wang and Liu [10]proposed a method of calculating the edge-Szeged index ofhexagonal chain.

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

EDGE SZEGEDINDEX

Theorem 1. $Sz_e(I_r(F_n)) = r^2(2n^2+4n-1) + r(6n^2+n-10) + (4n^2-5n-2)$.

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. Using the definition ofedge Szeged index, we have

$$Sz_e(I_r(F_n)) = \sum_{i=1}^{r}(m_v(vv^i)m_{v^i}(vv^i)) + \sum_{i=1}^{n}(m_v(vv_i)m_{v_i}(vv_i)) + \sum_{i=1}^{n-1}(m_{v_i}(v_iv_{i+1})m_{v_{i+1}}(v_iv_{i+1})) + \sum_{i=1}^{n}\sum_{j=1}^{r}(m_{v_i}(v_iv_i^j)m_{v_i^j}(v_iv_i^j))$$

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

$$(n-4)(2n+nr-2r-5)(r+2)) + (2(r+1)(2r+3) + 2(2r+2)(2r+3) + (n-4)(2r+3)(2r+3)) + nr(2n+r+nr-2)$$

$$= r^2(2n^2+4n-1) + r(6n^2+n-10) + (4n^2-5n-2). \square$$

Corollary 1. $Sz_e(F_n) = 4n^2-5n-2$.

Theorem 2. $Sz_e(I_r(W_n)) = r^2(2n^2+4n+1) + r(6n^2+4n-1) + (4n^2-n)$.

Proof. Let $C_n=v_1v_2\ldots v_n$and v_i^1, $v_i^2,\ldots$, 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 Szeged index, we infer

$$Sz_e(I_r(W_n))=\sum_{i=1}^{r}(m_v(vv^i)m_{v^i}(vv^i))+\sum_{i=1}^{n}(m_v(vv_i)m_{v_i}(vv_i))+\sum_{i=1}^{n}(m_{v_i}(v_iv_{i+1})m_{v_{i+1}}(v_iv_{i+1}))+\sum_{i=1}^{n}\sum_{j=1}^{r}(m_{v_i}(v_iv_i^j)m_{v_i^j}(v_iv_i^j))$$

$$=r(2n+r+nr-1)+n(r+2)(2n+nr-2r-5)+n(2r+3)(2r+3)+nr(2n+r+nr-1)$$

$$=r^2(2n^2+4n+1)+r(6n^2+4n-1)+(4n^2-n)\ .\ \square$$

Corollary 2. $Sz_e(W_n)=4n^2-n$.

Theorem 3. $Sz_e(I_r(\tilde{F}_n))=r^2(22n^2-43n+28)+r(45n^2-123n+84)+(18n^2-60n+46)$.

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, $v_i^2,\ldots$, v_i^r be the r hanging vertices of vi $(1 \le i \le n)$. Let $v_{i,i+1}^1$, $v_{i,i+1}^2,\ldots$, $v_{i,i+1}^r$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 edge Szeged index, we yield

$$Sz_e(I_r(\tilde{F}_n))=\sum_{i=1}^{r}(m_v(vv^i)m_{v^i}(vv^i))+\sum_{i=1}^{n}(m_v(vv_i)m_{v_i}(vv_i))+\sum_{i=1}^{n}\sum_{j=1}^{r}(m_{v_i}(v_iv_i^j)m_{v_i^j}(v_iv_i^j))$$

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

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

$$=r(3n+2nr-3)+(2(2r+1)(2nr+3n-2r-5)+(n-2)(3r+2)(2nr+3n-3r-7))+nr(3n+2nr-3)+$$

$$(n-1)(3r+2)(2nr-3r+3n-7)+(n-1)(3r+2)(2nr-3r+3n-7)+(n-1)r(3n+2nr-3)$$

$$=r^2(22n^2-43n+28)+r(45n^2-123n+84)+(18n^2-60n+46)\ .\ \square$$

Corollary3. $Sz_e(\tilde{F}_n)=18n^2-60n+46$.

Theorem 4. $Sz_e(I_r(\tilde{W}_n))=r^2(22n^2-14n+1)+r(45n^2-56n-1)+(18n^2-30n)$.

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, $v_i^2,\ldots$, 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 $v_{i,i+1}^1$, $v_{i,i+1}^2,\ldots$, $v_{i,i+1}^r$ 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 Szeged index, we deduce

$$Sz_e(I_r(\tilde{W}_n))=\sum_{i=1}^{r}(m_v(vv^i)m_{v^i}(vv^i))+\sum_{i=1}^{n}(m_v(vv_i)m_{v_i}(vv_i))+\sum_{i=1}^{n}\sum_{j=1}^{r}(m_{v_i}(v_iv_i^j)m_{v_i^j}(v_iv_i^j))$$

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

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

$$=r(2nr+3n+r-1)+n(3r+2)(2nr+3n-2r-5)+nr(2nr+3n+r-1)+n(3r+2)(2nr+3n-2r-5)+$$

$$n(3r+2)(2nr+3n-2r-5)+nr(2nr+3n+r-1)$$

$$=r^2(22n^2-14n+1)+r(45n^2-56n-1)+(18n^2-30n).\ \square$$

Corollary 4. $Sz_e(\tilde{W}_n)=18n^2-30n$.

DISCUSSIONS

In the definition of edge Szeged index, the notations $m_u(e)$ and $m_v(e)$ can be restated as

$$m_u(e)=\left|\{f\in E(G)\,|\,d'(f,u)<d'(f,v)\}\right|$$

and

$$m_v(e)=\left|\{f\in E(G)\,|\,d'(f,u)>d'(f,v)\}\right|,$$

where d' is defined as: If $f=xy\in E(G)$ and $u\in V(G)$, then $d'(f,u)=\min\{d(x,u),d(y,u)\}$.
The second edge-Szeged index was defined by Iranmanesh [11] as follows:

$$Sz'_e(G)=\sum_{e=uv}m'_u(e)m'_v(e),$$

where

$$m'_u(e)=\left|\{f\in E(G)\,|\,d'''(f,u)<d'''(f,v)\}\right|$$

and

$$m'_v(e)=\left|\{f\in E(G)\,|\,d'''(f,u)>d'''(f,v)\}\right|.$$

Also, d''' is

$$d'''(f,u)=\begin{cases}d''(f,u), & \text{if } u \text{ is not in } f\\ 0, & \text{if } u \text{ is in } f\text{, or } f=uv\end{cases}$$

where if $f=xy\in E(G)$ and $u\in V(G)$, then $d''(f,u)=\max\{d(x,u),d(y,u)\}$.

There few papers contribute to determine the second edge-Szeged index of molecular graphs. Hence, such modified index should be studied in the further.

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