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Edge-Szeged and vertex-PI indices of Some Benzenoid Systems

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Abstract. The edge version of Szeged index and vertex version of PI index are defined very recently. They are similar to edge-PI and vertex-Szeged indices, respectively. The different versions of Szeged and PI indices are the most important topological indices defined in Chemistry. In this paper, we compute the edge-Szeged and vertex-PI indices of some important classes of benzenoid systems.

Keywords: Edge and Vertex-Szeged indices, Edge and Vertex-PI indices, Benzenoid Systems.

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1. Introduction

Let G be a simple molecular graph with the vertex set $V(G)$ and the edge set $E(G)$. A topological index of G is a numeric quantity, derived following certain rules in Chemistry, which can be used to characterize the property of molecule.

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Usage of topological indices in Biology and Chemistry began in 1947 when chemist Harold Wiener1 introduced Wiener index to demonstrate correlations between physico-chemical properties of organic compounds of molecular graphs. The Wiener number is sum of distances between all unordered pairs of vertices of a simple graph G.

Khadikar and co-authors[2−5] defined a new topological index and named it Padmakar-Ivan index and they abbreviated this new topological index as PI. This was the edge version of PI index and defined as

$$PI_e(G) = \sum_{e=uv\in E(G)} [m_1(e\,|G) + m_2(e\,|G)]$$

where $m_1(e\,|G)$ is the number of edges of G which are closer to u than to v and $m_2(e\,|G)$ is the number of edges of G which are closer to v than to u. The various ways for computation of this index have been introduced for many graphs[6−7].

Quite recently the vertex version of PI index was also considered[8]. It is defined as $PI_v(G) = \sum_{e=uv\in E(G)}[n_1(e\,|G)+n_2(e\,|G)]$, such that $n_1(e\,|G)$ is the number of vertices of G which are closer to u than to v and $n_2(e\,|G)$ is the number of vertices of G which are closer to v than to u.

Another topological index was introduced by Gutman and called the Szeged index, abbreviated as Sz[9]. The Szeged index is a modification of Wiener index to cyclic molecules. This was the vertex version of Sz index which had been defined as $Sz_v(G) = \sum_{e=uv\in E(G)} n_1(e\,|G).n_2(e\,|G)$ where $n_1(e\,|G)$ and $n_2(e\,|G)$ have defined in above. In [10−12], you can find computations of this index for some graphs.

The edge version of Szeged index introduced very recently by Gutman and Ashrafi[13] that it is defined as $Sz_e(G) = \sum_{e=uv\in E(G)} m_1(e\,|G).m_2(e\,|G)$ where $m_1(e\,|G)$ and $m_2(e\,|G)$ have defined in up.

In this paper, we computed the vertex-PI and edge-Sz indices of $K^{n,n}$ and $T^{b,a}$ hexagonal systems.

2. Hexagonal system $K^{n,n}$

Shiu[14] defined a new hexagonal system named jagged-rectangle. An $n \times m$ hexagonal jagged-rectangle whose shape forms a rectangle and the number of hexagonal cells in each chain alternate n and $n-1$. For $n \geq 2$, the vertex set of $K^{n,m}$ defined as

$$V(K^{n,m}) = \{(x,y)\Big|0 \leq x \leq 2n, 0 \leq y \leq 2m-1\} \bigcup \{\{x,-1)\Big|0 \leq x \leq 2n-1\} \bigcup \{(x,2m)\Big|1 \leq x \leq 2n-1\}.$$

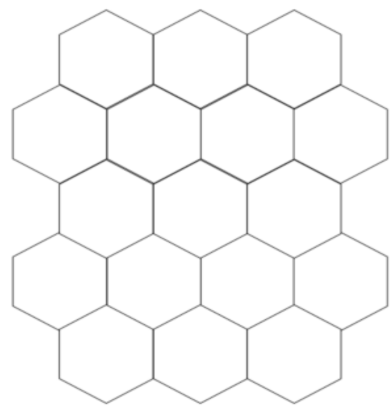

FIGURE 1. The graph $K^{4,2}$

One can see that $K^{n,n}$ has exactly $|V(K^{n,n})| = V = 4n^2 + 2n - 1$ vertices and $|E(K^{n,n})| = E = 6n^2 + 2n - 2$ edges.

2.1. **Vertex-PI index of $K^{n,n}$ hexagonal system.** To compute the vertex-PI index of $K^{n,n}$, we consider two types of edges, vertical and oblique. We denote the set of vertical edges with$A$and the set of oblique edges with B.

Lemma 2.1. *We have for the set A:* $\sum_{e\in A}[n_1(e\,|G)+n_2(e\,|G)] = \sum_{i=0}^{n} nV + \sum_{i=1}^{n}(n+1)V$.

Proof. According to the Figure 1, in the set$A$, we have n rows with $n+1$ vertical edges and $n+1$ rows with n vertical edges.

i) For rows which have n vertical edges, let $e = uv \in A$ and u be the up vertex of e. Then, we have: $n_1(e\,|G) = a_i = (2n-1)(i+1)+i(2n+1)+2i$ and $n_2(e\,|G) = V - a_i$.

ii) For rows which have $n+1$ vertical edges, let $e = uv \in A$ and u be the up vertex of e. Then, we have: $n_1(e\,|G) = b_i = 2i(2n+1) - 2$ and$n_2(e\,|G) = V - b_i$.

Therefore, we have for set A:

$$\begin{aligned}\sum_{e\in A}[n_1(e\,|G) + n_2(e\,|G)] &= \sum_{i=0}^{n} n(a_i + (V - a_i)) + \sum_{i=1}^{n}(n+1)(b_i + (V - b_i)) \\ &= \sum_{i=0}^{n} nV + \sum_{i=1}^{n}(n+1)V.\end{aligned}$$

□

Lemma 2.2. *We have for the set B:*

$$\sum_{e\in B}[n_1(e\,|G)+n_2(e\,|G)]=4\sum_{i=0}^{n-2}(2i+3)V+4nV.$$

Proof. According to the Figure 1, there exist two parts of oblique edges which are symmetric together. Then, at first, we compute above summation on one part and at last, we multiply 2 to this summation.
If $e=uv$ is an edge in one part and u is up vertex of e. Then:

$$n_1(e\,|G)=s_i=\sum_{k=0}^{i}(4k+5) \quad \text{and} \quad n_2(e\,|G)=V-s_i.$$

Therefore, we have for set B:

$$\begin{aligned}\sum_{e\in B}[n_1(e\,|G)+n_2(e\,|G)] &= 4\sum_{i=0}^{n-2}(2i+3)(s_i\\ &+(V-s_i))+4n(s_{n-2}+4n-1+(V-s_{n-2}-4n+1))\\ &=4\sum_{i=0}^{n-2}(2i+3)V+4nV.\end{aligned}$$

□

Theorem 2.3. *The vertex-PI index of $K^{n,n}$ hexagonal system is:*

$$PI_v(K^{n,n})=\sum_{e=uv\in E(K^{n,n})}[n_1(e\,|K^{n,n})+n_2(e\,|K^{n,n})]=12n^4+30n^3+5n^2-8n+1.$$

Proof. The proof is easy to check according to lemmas 2-1-1 and 2-1-2. □

2.2. **Edge-Szeged index of $K^{n,n}$ hexagonal system.** To compute the edge-Szeged index of $K^{n,n}$, we consider two types of edges, vertical and oblique, too. We denote the set of vertical edges with A and the set of oblique edges with B.

Lemma 2.4. *We have for the set A:*

$$\sum_{e\in A}m_1(e\,|G).m_2(e\,|G)=\sum_{i=0}^{n}na_i(E-a_i)+\sum_{i=1}^{n}(n+1)b_i(E-b_i).$$

Such that,

$$a_i=(2n-2)(i+1)+i(2n+2)+i(2n+1) \quad \textit{and} \quad b_i=4in+(i-1)(2n+1)+(n-2).$$

Proof. According to the Figure 1, in the set$A$, we have n rows with $n+1$ vertical edges and $n+1$ rows with n vertical edges.

iii) For rows which have n vertical edges, let $e = uv \in A$ and u be the up vertex of e. Then, we have: $m_1(e\,|G) = a_i = (2n-2)(i+1) + i(2n+2) + i(2n+1)$ and $m_2(e\,|G) = E - a_i$.

iv) For rows which have $n+1$ vertical edges, let $e = uv \in A$ and u be the up vertex of e. Then, we have: $m_1(e\,|G) = b_i = 4in+(i-1)(2n+1)+(n-2)$ and$m_2(e\,|G) = E - b_i$.

Therefore, we have for the set A:

$$\sum_{e\in A} m_1(e\,|G).m_2(e\,|G) = \sum_{i=0}^{n} na_i(E-a_i) + \sum_{i=1}^{n}(n+1)b_i(E-b_i).$$

□

Lemma 2.5. *We have for the set B:*

$$\sum_{e\in B} m_1(e\,|G).m_2(e\,|G) = 4\sum_{i=0}^{n-2}(2i+3)s_i(E-s_i)+4n(s_{n-2}+6n-3)(E-s_{n-2}-6n+3).$$

Such that, $s_i = \sum_{k=0}^{i}(10k+5) - 1$.

Proof. According to the Figure 1, there exist two parts of oblique edges which are symmetric together. Then, at first, we compute above summation on one part and at last, we multiply 2 to this summation.
We can cover every of these parts with $(2n-1)$-classes of parallel edges such that $(2n-2)$-classes of edges are two by two symmetric. Let $e = uv$ be an edge in one part and $u$be up vertex of e. The parallel edges of e have the same $m_1(e\,|G)$ and $m_2(e\,|G)$. Then: $m_1(e\,|G) = s_i = \sum_{k=0}^{i}(10k+5) - 1$ and $m_2(e\,|G) = E - s_i$.
Therefore, we have for set B:

$$\sum_{e\in B} m_1(e\,|G).m_2(e\,|G) = 4\sum_{i=0}^{n-2}(2i+3)s_i(E-s_i)+4n(s_{n-2}+6n-3)(E-s_{n-2}-6n+3).$$

□

Theorem 2.6. *The edge-Szeged index of $K^{n,n}$ hexagonal system is:*

$$\begin{aligned} Sz_e(K^{n,n}) &= \sum_{e=uv\in E(K^{n,n})} m_1(e\,|K^{n,n}).m_2(e\,|K^{n,n}) \\ &= \frac{116}{3}n^6 + 56n^5 + \frac{31}{3}n^4 - \frac{548}{3}n^3 + \frac{253}{2}n^2 - \frac{11}{6}n - 4. \end{aligned}$$

Proof. The proof is easy to check according to lemmas 2-2-1 and 2-2-2. □

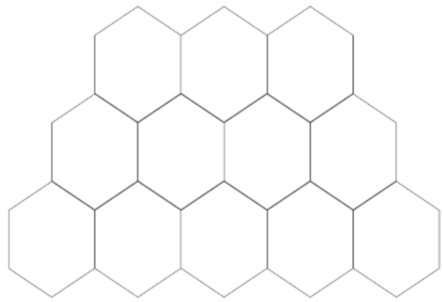

FIGURE 2. The graph $T^{3,5}$

3. HEXAGONAL SYSTEM $T^{b,a}$

A hexagonal trapezoid $T^{b,a}$ is a hexagonal system consisting $a-b+1$ rows of benzenoid chain in which every row has exactly one hexagon less than the immediate row, Figure 2.
The number of vertices of $T^{b,a}$ is equal to $\left|V(T^{b,a})\right| = V = a^2 - b^2 + 2a + 1$ and the number of edges of $T^{b,a}$ is equal to $\left|E(T^{b,a})\right| = E = \frac{3}{2}(a^2 - b^2) + \frac{5}{2}a - \frac{1}{2}b$.

3.1. **Vertex-PI index of $T^{b,a}$ hexagonal system.** Similar to calculation in section 2-1, we consider two separate classes A and B of vertical and oblique edges, respectively.

Lemma 3.1. *We have for the set A:* $\sum_{e\in A}[n_1(e\,|G) + n_2(e\,|G)] = \sum_{i=0}^{a-b}(b+i+1)V$.

Proof. Let $e = uv$ be a fix edge of A and u be the up vertex of e. Then:

$$n_1(e\,|G) = a_i = 2b(i+1) + 2i + 1 \quad \text{and} \quad n_2(e\,|G) = V - a_i.$$

And we have $b+i+1$ vertical edges in row, such that $0 \le i \le a-b$.
Therefore,

$$\sum_{e\in A}[n_1(e\,|G) + n_2(e\,|G)] = \sum_{i=0}^{a-b}(b+i+1)(a_i + (V - a_i)) = \sum_{i=0}^{a-b}(b+i+1)V.$$

□

Lemma 3.2. *We have for set B:*

$$\sum_{e\in B}[n_1(e\,|G) + n_2(e\,|G)] = 2(\sum_{i=1}^{b}(a-b+2)V + \sum_{i=0}^{a-b-1}(2+i)V).$$

Proof. According to the Figure 2, we can divide to two classes of oblique edges for the set B such that the summation of $n_1(e\,|G) + n_2(e\,|G)$ on edges of each part is equal together. Then, at first, we compute this summation on one part and at last, we multiply 2 to this summation. We have b oblique rows with $a-b+1$ hexagonal and $a-b$ oblique rows with less than $a-b+1$ hexagonal. Therefore,

i) Let $e=uv$ be a fix oblique edge of b oblique rows and u be the up vertex of e. Then, $n_1(e\,|G)=b_i=(2(a-b+1)+1)i$ and $n_2(e\,|G)=V-b_i$.
ii) Let $e=uv$ be a fix oblique edge of b oblique rows and u be the below vertex of e. Then, $n_1(e\,|G)=s_i=\sum_{k=0}^{i}(2k+3)$ and $n_2(e\,|G)=V-s_i$.

Therefore, we have:

$$\begin{aligned}\sum_{e\in B}[n_1(e\,|G)+n_2(e\,|G)] &= 2(\sum_{i=1}^{b}(a-b+2)(b_i+(V-b_i))\\ &\quad+\sum_{i=0}^{a-b-1}(2+i)(s_i+(V-s_i)))\\ &= 2(\sum_{i=1}^{b}(a-b+2)V+\sum_{i=0}^{a-b-1}(2+i)V).\end{aligned}$$

□

Theorem 3.3. *The vertex-PIindex of $T^{b,a}$ hexagonal system is:*

$$\begin{aligned}PI_v(T^{b,a}) &= \sum_{e=uv\in E(T^{b,a})}[n_1(e\,|T^{b,a})+n_2(e\,|T^{b,a})]\\ &= \frac{3}{2}(a^4+b^4)-3a^2b^2+\frac{15}{2}a^3-\frac{1}{2}b^3-\frac{15}{2}ab^2\\ &\quad+\frac{1}{2}ba^2+ba+\frac{23}{2}a^2-\frac{5}{2}b^2+\frac{1}{2}b+\frac{13}{2}a+1.\end{aligned}$$

Proof. The proof is easy to check according to lemmas 3-1-1 and 3-1-2. □

3.2. **Edge-Szeged index of $T^{b,a}$ hexagonal system.** Similar to calculation in above section, we consider two separate classes A and B of vertical and oblique edges, respectively.

Lemma 3.4. *We have for set A:*

$$\sum_{e\in A}m_1(e\,|G).m_2(e\,|G)=\sum_{i=0}^{a-b}(b+i+1)a_i(E-a_i).$$

Such that, $a_i=2b(i+1)+2i+r_i$ and $r_i=\sum_{k=1}^{i}(k+3)$.

Proof. Let $e=uv$be a fix edge of A and u be the up vertex of e. Then:
$m_1(e\,|G)=a_i=2b(i+1)+2i+r_i$ such that $r_i=\sum_{k=1}^{i}(k+b)$ and $m_2(e\,|G)=E-a_i$.
And we have $b+i+1$ vertical edges in row, such that $0\le i\le a-b$.
Therefore, $\sum_{e\in A}m_1(e\,|G).m_2(e\,|G)]=\sum_{i=0}^{a-b}(b+i+1)a_i(E-a_i)$. □

Lemma 3.5. *We have for the set B:*

$$\sum_{e\in B} m_1(e\,|G).m_2(e\,|G) = 2(\sum_{i=1}^{b}(a-b+2)b_i(E-b_i) + \sum_{i=0}^{a-b-1}(2+i)s_i(E-s_i)).$$

Proof. According to the Figure 2, we can divide to two classes of oblique edges for the set B such that the summation of $m_1(e\,|G).m_2(e\,|G)$ on edges of each part is equal together. Then, at first, we compute this summation on one part and at last, we multiply 2 to this summation. We have b oblique rows with $a-b+1$ hexagonal and $a-b$ oblique rows with less than $a-b+1$ hexagonal. Therefore,

iii) Let $e = uv$ be a fix oblique edge of b oblique rows and u be the up vertex of e. Then, $m_1(e\,|G) = b_i = 2i(a-b+1)+(a-b+2)(i-1)$ and $m_2(e\,|G) = E - b_i$.

iv) Let $e = uv$ be a fix oblique edge of b oblique rows and u be the below vertex of e. Then, $m_1(e\,|G) = s_i = \sum_{k=0}^{i}(2k+2) + \sum_{k=1}^{i}(k+2)$ and $m_2(e\,|G) = E - s_i$.

Therefore, we have:

$$\sum_{e\in B} m_1(e\,|G).m_2(e\,|G) = 2(\sum_{i=1}^{b}(a-b+2)b_i(E-b_i) + \sum_{i=0}^{a-b-1}(2+i)s_i(E-s_i)).$$

□

Theorem 3.6. *The vertex-PI index of $T^{b,a}$ hexagonal system is:*

$$\begin{aligned} Sz_e(T^{b,a}) &= \sum_{e=uv\in E(T^{b,a})} m_1(e\,|T^{b,a}).m_2(e\,|T^{b,a}) \\ &= \frac{25}{48}a^6 - \frac{109}{240}b^6 + \frac{7}{3}a^3b^3 + \frac{9}{16}a^2b^4 - \frac{57}{16}a^4b^2 \\ &+ \frac{3}{5}ba^5 + \frac{279}{80}a^5 - \frac{59}{80}b^5 + \frac{173}{8}a^2b^3 - \frac{217}{8}a^3b^2 - \frac{155}{48}ab^4 + \frac{287}{48}ba^4 + \frac{105}{16}a^4 \\ &+ \frac{63}{16}b^4 + \frac{367}{24}ba^3 + \frac{425}{24}ab^3 - \frac{87}{2}a^2b^2 + \frac{73}{16}a^3 - \frac{415}{48}b^3 - \frac{247}{48}ab^2 + \frac{187}{48}ba^2 \\ &+ \frac{71}{12}a^2 + \frac{91}{60}b^2 - \frac{223}{30}ab + \frac{19}{20}a + \frac{263}{60}b. \end{aligned}$$

Proof. The proof is easy to check according to lemmas 3-2-1 and 3-2-2. □

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