On the Szeged Index of some Benzenoid Graphs Applicable in Nanostructures

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Abstract

The Szeged index of a graph G is defined as $Sz(G) = \sum_{e=uv\in E(G)} N_u(e|G)N_v(e|G)$, where $N_u(e|G)$ is the number of vertices of G lying closer to u than to v and $N_v(e|G)$ is the number of vertices of G lying closer to v than to u. In this article, the Szeged index of some hexagonal systems applicable in nanostructures is computed.

Keywords. Benzenoid graphs, Szeged index, hexagonal system.

1. Introduction

A topological index is a real number related to a molecular graph. It must be a structural invariant, i.e., it does not depend on the labelling or the pictorial representation of a graph. The Wiener index W is the first topological index proposed in chemistry. It was introduced in 1947 by chemist Harold Wiener for characterization of alkanes. This index is defined as the sum of all distances between distinct vertices, see [18].

We now describe some notations where will be kept throughout. Benzenoid graphs, graph representations of benzenoid hydrocarbons, are

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defined as finite connected plane graphs with no cut-vertices, in which all interior regions are mutually congruent regular hexagons. Let G be a benzenoid graph. If all vertices of G lie on its perimeter, then G is said to be catacondensed; otherwise it is pericondensed. More details on this important class of molecular graphs can be found in the book of Gutman and Cyvin [7], and in the references cited therein.

Let G be a molecular graph possessing n vertices and m edges. If e is an edge of G, connecting the vertices u and v, then we write e = uv. If *G* is a connected graph and x and y are its two vertices, then the distance d(x,y) between the vertices x and y is equal to the length of the shortest path that connects them in G.

The Szeged index is a mathematically elegant topological index defined by Ivan Gutman at the Attila Jozsef University in Szeged, and so it was called the Szeged index, denoted by Sz. For more information about Szeged index we encourage the reader to consult [1-3,5,6,8-15,19,21] and references therein. To define we assume that G is a graph and e = uv is an edge of 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 vertices equidistant to u and v are not counted. Then the Szeged index of G is defined as $Sz(G) = \Sigma_{e\in E(G)} n_u(e)n_v(e)$.

Shiu, Tong and Lam [16] computed the Wiener index of three classes of benzenoid graphs named $I^{n,m}$, $J^{n,m}$ and $K^{n,m}$. In [20], the authors computed the Szeged index of these benzenoid graphs, for some special values of m and n. In this paper, we continue this work to compute the Szeged index of $I^{n,m}$, $J^{n,m}$ and $K^{n,m}$, for every positive integers m and n. All graphs considered are connected graphs. Our notation is standard and mainly taken from [4,17].

2. Main Results

In this section we extend the results of [20] on computing the Szeged index of $I^{n,m}$, $J^{n,m}$ and $K^{n,m}$. We first define these classes of benzenoid graphs. A hexagonal rectangle is called hexagonal jagged-rectangle, or simply HJR, if the number of hexagonal cells in each row is alternative between n and n − 1. Obviously, there are three types of HJR. If the top and bottom rows are longer we shall call it HJR of type I and denote by $I^{n,m}$. If the top and bottom rows are shorter we shall call it HJR of type K and denote by $K^{n,m}$. The last one is called HJR of type J and denoted by $J^{n,m}$. In the mentioned paper, Shiu, Tong and Lam computed the Wiener index of an arbitrary HJR, see [16] for details.

It is easy to see that $|V(I^{n,m})| = 2m(2n + 1)$, $|V(J^{n,m})| = 2m(2n+1) + (2n - 1)$, $|V(K^{n,m})| = 2m(2n + 1) + 2(2n - 1)$ and $|V(Q^{n,m})| = 2mn + 2m + 2n$. We also partition the set E(X), $X \in \{ I^{n,m}, J^{n,m}, K^{n,m}, Q^{n,m} \}$, into three subsets F, L_1 and L_2 as follows:

F = The set of all vertical edges,

L = The set of all oblique edges from left to right,

R = The set of all oblique edges from right to left.

Define $Sz_1(X) = \Sigma_{e=uv\in F} n_u(e)n_v(e)$, $Sz_2(X) = \Sigma_{e=uv\in L} n_u(e)n_v(e)$ and $Sz_3(X) = \Sigma_{e=uv\in R} n_u(e)n_v(e)$. It is clear that $Sz(X) = Sz_1(X) + Sz_2(X) + Sz_3(X)$ and by symmetry of X, $Sz_2(X) = Sz_3(X)$. Thus for computing Sz(X), it is enough to compute $Sz_1(X)$ and $Sz_2(X)$.

We now proceed to compute the Szeged index of the graph of $I^{n,m}$, Figure 1. To compute $Sz_1(G)$, we notice that there are 2m + 1 rows with vertical edges, see Figure 1. Define $\varepsilon: N \to \{0,1\}$ by $\varepsilon(i) = 1$, if i is odd, and 0 otherwise. We also assume that A and B are sets of all vertical edges lie in the long and small rows of this graph, respectively. Then $n_u^i(e)=(2n+1)i$ and $n_v^i(e)=(2n+1)(2m-i)a$ in which $n_u^i(e)$ denotes the number of vertices of G in the i^{th} row whose distance to the vertex u is smaller than the distance to the vertex v. Then the number of vertical edges in the i^{th} row is $\varepsilon(i) + n$ and we have:

$$Sz_1(I^{n,m}) = \sum_{i=1}^{2m-1}(\varepsilon(i)+n)i(2n+1)(2n+1)(2m-i)$$
$$=\frac{16}{3}m^3n^3 - \frac{4}{3}n^3m + \frac{2}{3}m^3 + \frac{m}{3} + 8n^2m^3 + 4nm^3 + nm.$$

To compute $Sz_2(I^{n,m})$, we consider two different cases as follows:

Case 1) $n \geq m$. Suppose k_i denotes the number of oblique edges from left to right in the i^{th} row. Suppose e = uv is an edge in the i^{th} row of $I^{n,m}$ then

$$k_i = \begin{cases} 2i & 1 \le i < m \\ 2m & m \le i < n \\ 2(n+m-i) & n \le i \le m+n \end{cases},$$

$$n_u^i(e) = \left(\sum_{s=Max\{1,i\}}^{m-1}(K_s + K_{s+1} + 1)\right) + \left(\sum_{s=Max\{i,m\}}^{n-1}(K_s + K_{s+1})\right) + \left(\sum_{s=Max\{i,n\}}^{n+m-1}(K_s + K_{s+1} + 1)\right),$$

and $n_v^i(e) = 2m(2n+1) - n_u^i(e)$. Therefore,

$$n_u^i(e) = \begin{cases} 2m^2 - 2i^2 - i + 4nm & 1 \le i < m \\ 4nm - 4im + 2m^2 + m & m \le i < n \\ 4mn + 2m^2 + 2n^2 + n + m + 4im - 4in + 2i^2 - i & n \le i \le m+n \end{cases}.$$

This implies that

$$n_v^i(e) = \begin{cases} 2i^2 + i & 1 \le i < m \\ m + 4im - 2m^2 & m \le i < n \\ m - 2m^2 - 2n^2 - n + 4im - 4in + 2i^2 - i & n \le i \le m+n \end{cases},$$

and so

$$15Sz_2(I^{n,m})=15\sum_{i=1}^{m+n-1} k_i n_u^i(e) n_v^i(e)$$
$$= 80m^3n^3 + 12m^5 - 40m^4n + 120m^3n^2 - 25m^4 + 70m^3n .$$
$$- 20m^3 + 40m^2n + 25m^2 + 8m.$$

Therefore,

$$15Sz(I^{n,m}) = 240m^3n^3 + 24m^5 - 80m^4n + 360m^3n^2 - 50m^4 +$$
$$200m^3n - 20mn^3 - 30m^3 + 80m^2n + 50m^2 + 15mn + 21m.$$

Case 2) $m \ge n$. In this case the number of oblique edges from left to right in the i^{th} row of $I^{n,m}$ and $n_u^i(e)$ are computed as

$$k_i = \begin{cases} 2i & 1 \le i < m \\ 2n & m \le i < n \\ 2(n+m-i) & n \le i \le m+n \end{cases},$$

$$n_u^i(e) = \left(\sum_{s=Max\{1,i\}}^{m-1} (K_s + K_{s+1} + 1) \right) + \left(\sum_{s=Max\{i,n\}}^{m-1} (K_s + K_{s+1} + 2) \right). + \left(\sum_{s=Max\{i,m\}}^{n+m-1} (K_s + K_{s+1} + 1) \right)$$

Using above calculations and some simple equations about the sum of successive integers and successive squares, one can see that

$$n_u^i(e) = \begin{cases} 4nm + 2m - 2i^2 - i & 1 \le i < m \\ 2n^2 + 4nm - 4in + n + 2m - 2i & m \le i < n \\ 4mn + 2m^2 + 2n^2 + n + m - 4im - 4in + 2i^2 - i & n \le i \le m+n \end{cases},$$

Hence

$$n_v^i(e) = \begin{cases} 2i^2 + i & 1 \le i < m \\ -2n^2 + 4in - n + 2i & m \le i < n \\ -2m^2 - 2n^2 - n + 4im + 4in + m - 2i^2 + i & n \le i \le m+n \end{cases}.$$

for $m \ge n$, $15Sz(I^{n,m}) = 15Sz_1(I^{n,m}) + 30Sz_2(I^{n,m}) = 240m^3n^3 + 15mn + 280m^3n^2 + 10m^3 - 40mn^2 + 50n^2 + 40mn^4 - 16n^5 + 100m^3n + 80mn^3 - 50n^4 + 5m + 16n$. Thus we proved the following theorem:

Theorem 1. The Szeged index of $I^{n,m}$ is computed as follows:

$$Sz(I^{n,m}) = \frac{1}{15} \times \begin{cases} 240m^3n^3 + 24m^5 - 80m^4n + 360m^3n^2 - 50m^4 + 21m & m \le n \\ +200m^3n - 20mn^3 - 30m^3 + 80m^2n + 50m^2 + 15mn & \\ 240m^3n^3 + 15mn + 280m^3n^2 + 10m^3 - 40mn^2 + 50n^2 + & n \le m \\ 40mn^4 - 16n^5 + 100m^3n + 80mn^3 - 50n^4 + 5m + 16n & \end{cases}$$

In particular case that $m = n$, $Sz(I^{n,n}) = (1/15)(240n^6 + 304n^5 + 130n^4 + 50n^3$ $65n^2 + 21n)$.

We now compute the Szeged index of $J^{n,m}$, Figure 2. To do this, we notice that according to vertical edges, there are 2m rows in which 1^{th}, 3^{th}, ..., $(2m-1)^{th}$ rows of the graph have exactly n+1 vertical edges and other rows have n vertical edges. On the other hand, if e = uv lie in the i^{th} row of $J^{n,m}$ then $n_u^i(e) = (2n+1)i$ and since $J^{m,n}$ is bipartite $n_v^i(e) = 2m(2n+1) + (2n-1) - n_u^i(e) = (2m-i)(2n+1) + 2n - 1$. Thus

$$\begin{aligned} 3Sz_1(J^{n,m}) &= 3\sum_{i=1}^{2m}(\varepsilon(i)+n)i(2n+1)[(2n+1)(2m-i)+2n-1] \\ &= 16m^3n^3 + 24m^3n^2 + 24m^2n^3 + 12m^3n + 12m^2n^2 \\ &\quad + 8mn^3 + 2m^3 + m - 3m^2 - 6nm^2. \end{aligned}$$

To compute $Sz_2(J^{n,m})$, we consider again two separate cases that $n \geq m$ or $n \geq m$.

Case 1) $n \geq m$. Suppose T_i denotes the number of edges from left to right in the i^{th} row of $J^{n,m}$. Then

$$T_i = \begin{cases} 2i & 1 \leq i \leq m \\ 2m+1 & m < i \leq n \\ 2(n+m-i)+1 & n < i \leq m+n \end{cases},$$

$$\begin{aligned} n_u^i(e) &= \left(\sum_{s=1}^{m}(T_s + T_{s+1} + 1)\right) \\ &\quad + \left(\sum_{s=m+1}^{n}(T_s + T_{s-1})\right) \\ &\quad + \left(\sum_{s=n+1}^{n+m-1}(T_s + T_{s-1} + 1)\right) \end{aligned},$$

and since $J^{n,m}$ is bipartite, $n_v^i(e) = 2m(2n+1) + (2n-1) - n_u^i(e)$. Using similar calculations as above,

$$n_u^i(e) = \begin{cases} 2i^2 + i & 1 \leq i \leq m \\ -2m^2 - m + 4im + 2i - 1 & m < i \leq n \\ -2m^2 - 2n^2 + 4im + 4in - m - n + 3i - 2i^2 - 1 & n < i \leq m+n \end{cases},$$

$$n_v^i(e) = \begin{cases} 4mn + 2m + 2n - 1 - i - 2i^2 & 1 \leq i \leq m \\ 2m^2 + 4mn + 3m - 4im + 2n - 2i & m < i \leq n \\ 2m^2 + 4mn + 2n^2 - 4im + 3m + 3n - 4in - 3i + 2i^2 & n < i \leq m+n \end{cases}.$$

Therefore,

$$\begin{aligned} 15Sz_2(J^{n,m}) &= 80m^3n^3 + 12m^5 - 40m^4n + 120m^3n^2 - 10m^4 + 20m^3n + 4m^2n^2 + 5n + \\ &\quad 60mn^3 - 45m^3 + 40m^2n - 30mn^2 + 10n^3 - 35n^2 + 20mn - 15n^2 - 12m, \end{aligned}$$

and so $15Sz(J^{n,m}) = 15Sz_1(J^{n,m}) + 30Sz_2(J^{n,m}) = 240m^3n^3 + 360m^3n^2 + 360m^2n^3 +$

$180m^2n^2 - 60mn^2 - 30n^2 + 24m^5 + 80m^4n - 20m^4 + 100m^3n + 160mn^3 - 80m^3 + 50m^2n + 20n^3 - 85m^2 + 40mn - 19m + 10n.$

Case 2) $m \geq n$. In this case, we have

$$T_i = \begin{cases} 2i & 1 \leq i \leq n \\ 2n & n < i \leq m \\ 2(n+m-i)+1 & m < i \leq m+n \end{cases},$$

$$\begin{aligned} n_u^i(e) &= \left(\textstyle\sum_{s=1}^{n} (T_s + T_{s+1} + 1) \right) \\ &+ \left(\textstyle\sum_{s=n+1}^{m} (T_s + T_{s-1} + 2) \right), \\ &+ \left(\textstyle\sum_{s=m+1}^{n+m-1} (T_s + T_{s-1} + 1) \right) \end{aligned}$$

$n_v^i(e) = 2m(2n+1) + (2n-1) - n_u^i(e),$

$$n_u^i(e) = \begin{cases} 2i^2 + i & 1 \leq i \leq n \\ -2n^2 - n + 4in + 2i & n < i \leq m \\ -2m^2 - 2n^2 + 4im + 4in - m - n + 3i - 2i^2 - 1 & m < i < m+n \end{cases},$$

$$n_v^i(e) = \begin{cases} 4mn + 2m + 2n - 1 - i - 2i^2 & 1 \leq i \leq n \\ 2n^2 + 4mn + 3n - 4in + 2m - 1 - 2i & n < i \leq m \\ 2m^2 + 4mn + 2n^2 - 4im + 3m + 3n - 4in - 3i + 2i^2 & m < i < m+n \end{cases},$$

and so $15Sz(J^{n,m}) = 15Sz_1(J^{n,m}) + 30Sz_2(J^{n,m}) = 240m^3n^3 + 360m^2n^3 + 60m^2n^2 - 60n^4 - 90m^2n + 60n^3 - 15m^2 - 90mn + 30n^2 + 280m^3n^2 + 40mn^4 - 16n^5 + 100m^3n + 320mn^3 + 30m^3 - 50mn^2 + 5m - 14n.$

We now ready to state our second result.

Theorem 2. The Szeged index of $J^{n,m}$ is computed as follows:

$$Sz(J^{n,m}) = \frac{1}{15} \cdot \begin{cases} 240m^3n^3 + 360m^3n^2 + 360m^2n^3 + 180m^2n^2 - 60mn^2 & m \leq n \\ - 30n^2 + 24m^5 + 80m^4n - 20m^4 + 100m^3n + 160mn^3 & \\ -80m^3 + 50m^2n + 20n^3 - 85m^2 + 40mn - 19m + 10n & \\ & \\ 240m^3n^3 + 360m^2n^3 + 60m^2n^2 - 60n^4 - 90m^2n + & n \leq m \\ 60n^3 - 15m^2 - 90mn + 30n^2 + 280m^3n^2 + 40mn^4 - 16n^5 & \\ +100m^3n + 320mn^3 + 30m^3 - 50mn^2 + 5m - 14n & \end{cases}$$

In the case of $m = n$, $Sz(J^{n,n}) = (1/15)(240n^6 + 664n^5 + 360n^4 - 70n^3 - 75n^2 - 9n)$.

We now compute the Szeged index of the graph $K^{n,m}$, Figure 3. By a similar calculations as those of Theorems 1 and 2, one can see that

$3Sz_1(K^{n,m}) = 16m^3n^3 + 24m^3n^2 + 36m^2n^3 + 12m^3n + 24m^2n^2 + 20mn^3 + 2m^3 - 9m^2n - 6m^2 - 9mn + 4m$, and

$$Sz_2(K^{n,m}) = \frac{1}{15}\cdot\begin{cases} 80m^3n^3+12m^5n-40m^4n+120m^3n^2+240m^2n^3+ & n>m \\ 5m^4-30m^3n+120m^2n^2+240mn^3+70n-70m^3+ & \\ 10m^2n-120mn^2+80n^3-140m^2+70mn-120n^2 & \\ -107m-30 & \\ & \\ 80m^3n^3-8n^5+20mn^5+240m^2n^3+80m^3n^2-35n^4 & n\le m \\ +350mn^3+20m^3n+150n^3-190mn^2-60m^2n- & \\ 130n^2-60mn+23n & \end{cases}$$

Therefore we can state the following theorem:

Theorem 3. The Szeged index of $K^{n,m}$ is computed as follows:

$$Sz(K^{n,m}) = \frac{1}{15}\cdot\begin{cases} 240m^3n^3+280m^3n^2+720m^2n^3+40mn^4-16n^5+100m^3n & m\ge n \\ +120m^2n^2+920mn^3-70n^4+10m^3-180m^2n-440mn^2 & \\ +360n^3-30m^2-165mn-960n^2+20m+61n & \\ & \\ 240m^3n^3+24m^5-80m^4n+360m^3n^2+720m^2n^3+10m^4 & m<n \\ +360m^2n^2+700mn^3-130m^3-40m^2n-300mn^2+ & \\ 220n^3-310m^2+95mn-300n^2-194m+155n-60 & \end{cases}$$

In particular, $Sz(K^{n,n}) = (1/15)(240n^6 + 1024n^5 + 1070n^4 - 250n^3 - 515n^2 + 81n)$.

Finally, we compute the Szeged index of the graph $Q^{n,m}$, Figure 4. Using a similar argument as above, one can see that $3Sz_1(Q^{n,m}) = m + 3mn + 6m^2n + 12m^2n^2 + 6mn^2 + 4mn^3 + 2m^3n^3 + 6m^3n^2 - 6m^3n + 6m^2n^3 + 2m^3$ and

$$6Sz_2(Q^{n,m}) = \begin{cases} 4m^3n^3+12m^3n^2+12n^3m^2+12nm^3+24m^2n^2+ & m\ge n \\ 14mn^3-n^4+4m^3+12m^2n+2n^3+n^2-4m-2n & \\ & \\ 4m^3n^3+12m^3n^2+12n^3m^2-m^4+14nm^3+24m^2n^2 & m<n \\ +12mn^3+2m^3+18m^2n+12mn^2+4n^3+m^2-2m-4n & \end{cases}$$

We are now ready to state our final theorem as follows:

Theorem 4. The Szeged index of $Q^{n,m}$ is computed as follows:

$$Sz(Q^{n,m}) = \frac{1}{6}\cdot \begin{cases} 12m^3n^3 + 36m^3n^2 + 36n^3m^2 + 36nm^3 + 72m^2n^2 + 36mn^3 - 2n^4 & m \geq n \\ +12m^3 + 36m^2n + 48mn^2 + 4n^3 + 6m + 2n^2 - 6m - 4n & \\ & \\ 12m^3n^3 + 36m^3n^2 + 36n^3m^2 - 2m^4 + 40nm^3 + 72m^2n^2 + 32mn^3 & m < n \\ +8m^3 + 48m^2n + 36mn^2 + 8n^3 + 2m^2 + 6mn - 2m - 8n & \end{cases}$$

In particular, $Sz(Q^{n,n}) = (1/3)(6n^6 + 36n^5 + 71n^4 + 50n^3 + 4n^2 - 5n)$.

In the case that $m = (n + 1)/2$, we can deduce some of the results in [19] by Theorems 1-4.

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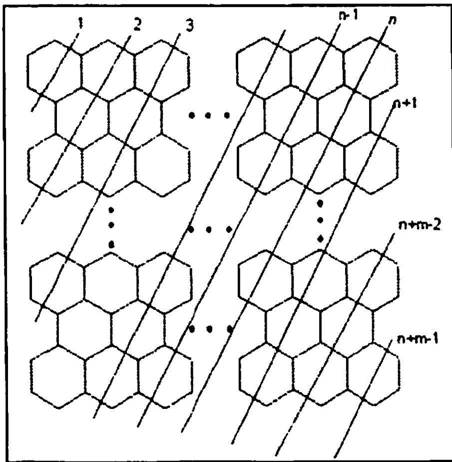

Figure 1. The Graphs of $I^{n,m}$.

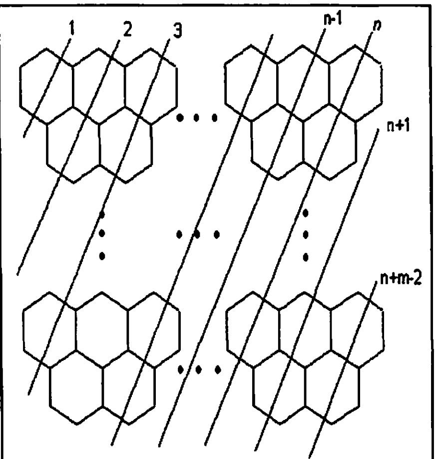

Figure 2. The Graphs of $J^{n,m}$.

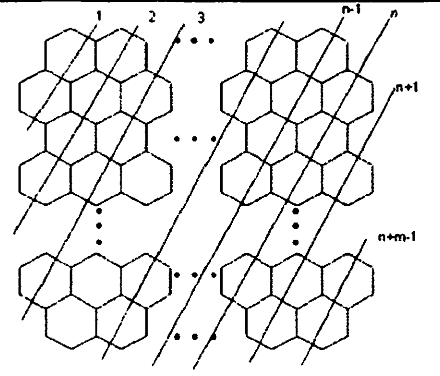

Figure 3. The Graphs of $K^{n,m}$.

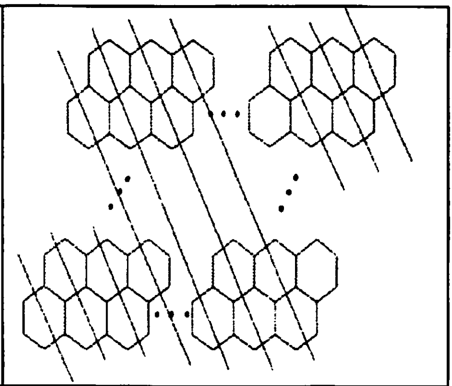

Figure 4. The Graphs of $Q^{n,m}$.

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