PI and Szeged Indices of some Benzenoid Graphs Related to Nanostructures

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Abstract

In this paper, we compute the PI and Szeged indices of some important classes of benzenoid graphs, which some of them are related to nanostructures. Some open questions are also included.

Keywords: PI index, Szeged index, benzenoid graph, topological index.

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 oldest topological indices of a molecular graph G is the Wiener index W = W(G). This index is defined as the sum of distances between distinct vertices and was introduced by chemist Harold Wiener, [23]. In the 1990s, a large number of other topological indices have been put forward, all being based on the distances between vertices of molecular graphs and all being closely related to W. Szeged index is one of these topological indices, which is introduced by Ivan Gutman, see [9,10,18]. To define the Szeged index of a graph G, we assume that e = uv is an edge connecting the vertices u and v.

Suppose $N_u(e|G)$ is the number of vertices of G lying closer to u and $N_v(e|G)$ is the number of vertices of G lying closer to v. Edges equidistance from u and v are not taken into account. Then the Szeged index of G is defined as $Sz(G) = \sum_{e=uv\in E(G)} N_u(e|G)N_v(e|G)$.

A Szeged-like topological index introduced very recently by P V. Khadikar, [13-16]. It is defined as the sum of $[n_u(e|G) + n_v(e|G)]$ between all edges e=uv of a graph G: $PI(G) = \sum_{e\in G}[n_{eu}(e|G)+ n_{ev}(e|G)]$, where $n_u(e|G)$ is the number of edges of G lying closer to u than to v and $n_v(e|G)$ is the number of edges of G lying closer to v than to u. Mathematical properties of the PI index for some classes of chemical graphs can be found in recent papers, [1-6,8,19,24].

We now describe some notations which will be kept throughout. Benzenoid systems (graph representations of benzenoid hydrocarbons) are defined as finite connected plane graphs with no cut-vertices, in which all interior regions are mutually congruent regular hexagons. More details on this important class of molecular graphs can be found in the book of Gutman and Cyvin [10], and in the references cited therein.

In this paper we only consider connected graphs. Our notation is standard and mainly taken from [7,10,22].

2. Results and Discussion

Let G be a benzenoid graph. If all of vertices of the graph G lie on its perimeter, then G is said to be catacondensed; otherwise it is pericondensed. In this section we calculate the PI and Szeged indices of some benzenoid graphs and present some open questions.

Definition 1. Suppose G is a hexagonal system, e = xy, f = uv $\in$ E(G) and w $\in$ V(G). Define $d(w,e) = Min\{d(w,x) , d(w,y)\}$. We say that e is parallel to f if $d(x,f) = d(y,f)$ and we write $e \parallel f$.

Lemma 1. || is a reflexive and symmetric relation, but it is not transitive.

Proof. Reflexivity is trivial. To prove || is symmetric, we assume that e = xy is parallel to f = uv. By definition d(x,f) = d(y,f). If d(x,u) = d(x,v) then we obtain a cycle of odd length containing the edge f, a contradiction. Hence d(x,u) ≠ d(x,v) and similarly d(y,u) ≠ d(y,v). Without loss of generality we can assume that d(x,u) < d(x,v). Then by assumption d(y,v) < d(y,u) and we can see that d(x,u) = d(y,v), d(x,v) = d(y,u). On the other hand, d(x,u) < d(x,v) and d(y,v) < d(y,u) imply that d(x,v) = d(x,u) + 1 and d(y,u) = d(y,v) + 1. This shows that d(u,e) = Min{d(u,x),d(u,y)} = Min{d(x,v) - 1,d(y,v) + 1} = Min{d(y,u) – 1, d(x,u) + 1} = Min{d(y,v),d(x,v)} = d(v,e), as desired. Finally, we show that || is not transitive. To do this, we consider the graph of a polyhex nanotorus with p = 2 and q = 6, Figure 1. In this graph, e||f and f||g but e is not parallel to g. □

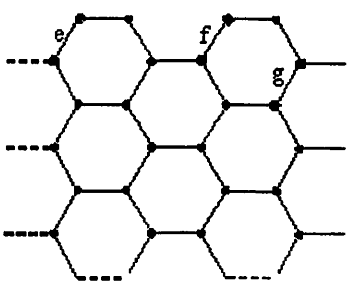


Figure 1. A Polyhex Nanotorus with p=2 and q=6.

Question 1: Under what condition(s) is parallelism an equivalence relation?

Definition 2. Suppose G is a hexagonal system and e ∈ E(G). We define P(e) to be the set of all edges parallel to e and N(e) = |P(e)|.

It is clear that N(e) = |E| – (n_{eu}(e|G) + n_{ev}(e|G)), where e is an arbitrary edge of the graph G. Thus PI(G) = $|E|^2 - \sum_{e\in E(G)}$ N(e). We use this simple equation freely throughout the paper.

Example 1. Consider the hexagonal triangle graph G = T(n) of Figure 2, containing j hexagons in the j^{th} row, $1 \le j \le n$. This graph is related to the atomic structure of bipod shaped nanocrystals, see Figure 13 of [12]. Since the graph G has an equilateral figure, $|E(G)| = 3(2 + 3 + 4 + \ldots + (n + 1)) = 3/2(n^2 + 3n)$. On the other hand, an arbitrary edge e of the j^{th} row of T(n) has exactly j + 1 parallel edges and so $\sum_{e\in G} N(e) = 3[2^2 + 3^2 + \ldots + (n+1)^2] = 1/2[2n^3 + 18n^2 + 13n] = n^3 + 9n^2 + 13/2n$. Therefore,

$$PI(G) = |E|^2 - \sum_{e\in E(G)} N(e) = 1/4[9n^4 + 50n^3 + 63n^2 - 26n].$$

We now compute the Szeged index of this graph. Obviousely, $|V(G)| = 3 + 5 + \ldots + (2n+1) = n^2 + 4n + 1$. Consider a vertical edge e = uv of the j^{th} row of the graph T(n). We note that this row has exactly j + 1 vertical edges and so $S_j = N_u(e|G) = [3 + 5 + \ldots + (2j - 1)] = j^2 + 2j$ and $T_j = N_v(e|G) = n^2 + 4n + 1 - j^2 - 2j$. Therefore,

$$\begin{aligned} Sz(G) &= 3\sum_{1\le i\le n} N_u(e|G)N_v(e|G) \\ &= 3\sum_{1\le i\le n} (1+i)SiT_i \\ &= \sum_{1\le i\le n} [-i^5-5i^4+(n^2+4n-7)i^3+(3n^2+12n-1)i^2+2(n^2+4n+1)i] \\ &= 1/4[n^6 + 12n^5 + 49n^4 + 84n^3 + 58n^2 + 12n]. \end{aligned}$$

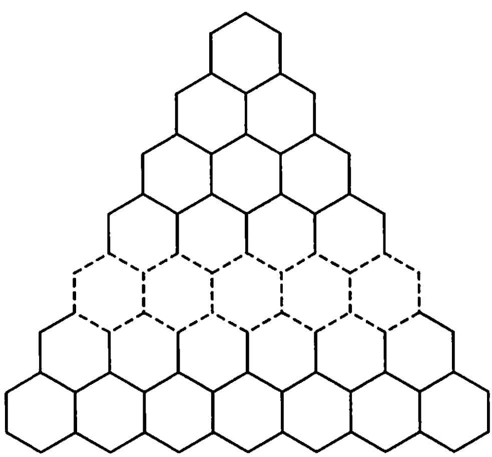


Figure 2. The Hexagonal Triangle Graph T(n)

Example 2. Let H_n be an n-hexagonal net, which is a hexagonal system consisting of one central hexagon and is surrounded by n−1 layers of hexagonal cells when $n \geq 1$, Figure 3. H_n is a molecular graph, corresponding to benzene (n=1), coronene (n=2) circumcoronene (n=3), circum–circumcoronene (n=4), etc. In [20], Shiu and Lam computed the Wiener index of an n-hexagonal net. They proved that $W(H_n) = 1/5(164n^5 - 30n^3 + n)$. Here the PI and Szeged indices of this graph are computed. Since the j^{th} row of the graph H_n has exactly n + j vertical edges, $|E(H_n)| = 3\{2[(n+1) + (n+2) + \ldots + (2n - 1)] + 2n\} = 9n^2 - 3n$. A similar calculation shows that $|V(G)| = 6n^2$. On the other hand, if e is an arbitrary edge of the j^{th} row of this graph, $1 \leq j \leq n-1$, then e has exactly n + j parallel edges and so

$$PI(H_n) = |E(H_n)|^2 - 3\{2\sum_{i=1}^{n-1}(n+i)^2 + 4n^2\}$$
$$= (9n^2 - 3n)^2 - (14n^3 - 3n^2 + n) = 81n^4 - 68n^3 + 12n^2 - n.$$

To compute the Szeged index of H_n, we consider a vertical edge e = uv in the j^{th} row of H_n. Then for an arbitrary vertex t of the i^{th} row of H_n, $d(t,u) < d(t,v)$ if and only if $i \leq j$. Suppose A is the set of all vertical edges of H_n. For n=1 $Sz(H_n) = 54$ and so it is enough to consider $n \geq 2$. If e = uv is a vertical edge in the i^{th} row, Figure 3, Then the number of vertices which are closer to u than v is as follows:

$$(2n+1) + (2n+3) + \ldots + (2n + 2i - 1) = 2ni + i^2.$$

Since H_n is symmetric, we have:

$$Sz(H_n) = 3\sum_{e=uv\in A} N_u(e|G)N_v(e|G)$$
$$= 3\{2\sum_{1\leq i\leq n-1} [(2ni+i^2)(n+i)(6n^2 - 2ni - i^2)] + 2n(3n^2)(3n^2)\}$$
$$= 54n^6 - 3/2n^4 + 3/2n^2.$$

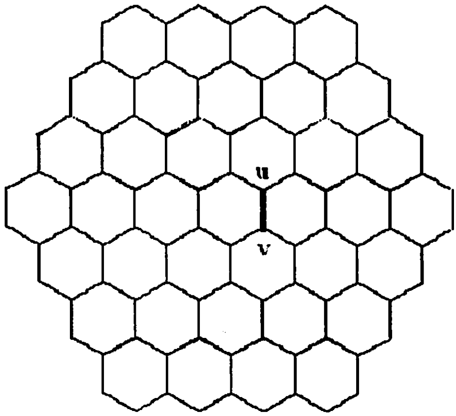


Figure 3. A 4–hexagonal net (circum-circumcoronene).

Example 3. A graph formed by a row of n hexagonal cells is called an n-hexagonal chain. A hexagonal parallelogram $Q_{n,m}$, is a graph containing m n-hexagonal chain in every row, Figure 4. Consider a hexagonal parallelogram $Q_{n,n}$ to compute its PI and Szeged indices. It is clear that $|E(Q_{n,n})| = 3n^2 + 4n - 1$ and $|V(Q_{n,n})| = 2n^2 + 4n$. This graph has three types of edges, vertical, left oblique and right oblique. Let A, B and C denote the set of all vertical, left oblique and right oblique edges of $Q_{n,n}$. Then $\sum_{e\in E(Q_{n,n})}N(e) = \sum_{e\in A}N(e) + \sum_{e\in B}N(e) + \sum_{e\in C}N(e)$ and we have:

$$\sum_{e\in A}N(e) = n(n+1)^2 = n^3 + 2n^2 + n,$$

$$\sum_{e\in B}N(e) = n(n+1)^2 = n^3 + 2n^2 + n,$$

$$\sum_{e\in C}N(e) = 2[2^2 + 3^2 + \ldots + n^2] + (n+1)^2$$

$$\sum_{e\in E(Q_{n,n})}N(e) = 1/3(8n^3 + 18n^2 + 13n - 3).$$

Hence $PI(Q_{n,n}) = |E(Q_n)|^2 - \sum_{e\in E(Q_{n,n})}N(e) = 1/3(27n^4 + 64n^3 + 12n^2 - 37n + 6)$. We now compute the Szeged index of this graph. To do this, we note that $Q_{n,n}$ has exactly three types of edges, say I, II and III. The edges of type I are vertical and the edges of type II and III are left and right oblique edges, respectively. It is easy to see that for an arbitrary edge e = xy of type I and an arbitrary edge f of type II, we have $N_x(e|Q_{n,n}) = N_u(f|Q_{n,n})$ and $N_y(e|Q_{n,n}) = N_v(f|Q_{n,n})$. Define $Sz_1 = 2\sum_{e=uv\in I} N_u(e|Q_{n,n})N_v(e|Q_{n,n})$ and $Sz_2 = \sum_{e=uv\in III} N_u(e|Q_{n,n})N_v(e|Q_{n,n})$. Then $Sz(Q_{n,n}) = Sz_1 + Sz_2$ and we have:

$$\begin{aligned} Sz_1 &= \sum_{e=uv\in I} N_u(e|Q_{n,n})N_v(e|Q_{n,n}) \\ &= (n+1)\sum_{0\le i\le n-1}[2n+1+i(2n+2)][2n^2+4n-2n-1-i(2n+2)], \\ &= 1/3(2n^6+12n^5+22n^4+14n^3+3n^2+n), \end{aligned}$$

To compute Sz_2, we choose $e_1 = x_1y_1$, $e_2 = x_2y_2$, ..., $e_n = x_ny_n$ to be the final left oblique edges of the 1^{th}, 2^{th} and etc row of $Q_{n,n}$. Then we have:

$$\begin{aligned} Sz_2 &= \sum_{e=uv\in III} N_u(e|Q_{n,n})N_v(e|Q_{n,n}), \\ &= 2\sum_{1\le i\le n}(1+i)N_{xi}(e_i|Q_{n,n})N_{yi}(e_i|Q_{n,n}) - (n+1)S_n^2 \\ &= 2\sum_{1\le i\le n}(1+i)S_i(2n^2+4n-S_i) - (n+1)S_n^2 \\ &= 1/6(4n^6+24n^5+49n^4+36n^3+n^2-6n), \end{aligned}$$

in which $S_i = 3 + 5 + \ldots + (2i+1) = i^2 + 2i$. Now $Sz(Q_{n,n}) = Sz_1(Q_{n,n}) + Sz_2(Q_{n,n})$ and so $Sz(Q_{n,n}) = 1/6(12n^6 + 72n^5 + 137n^4 + 92n^3 + 13n^2 - 2n)$.

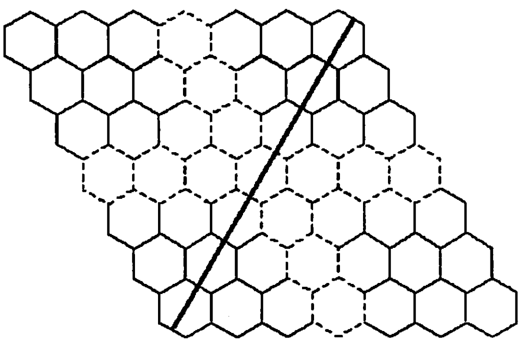


Figure 4. The Hexagonal Parallelogram $Q_{n,n}$.

Example 4. Following Shiu, Tong and Lam [23], 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 row are longer we shall call it HJR of type I and denoted by $I^{n,m}$. If the top and bottom row are shorter we shall call it HJR of type K and denoted by $K^{n,m}$. The last one is called HJR of type J and denoted by $J^{n,m}$.

In [21], Shiu, Tong and Lam computed the Wiener index of an arbitrary HJR. The exact expression for the Wiener index of an arbitrary HJR is lengthy to be included here. In what follows, we compute the PI and Szeged indices of hexagonal jagged-squares $G = I^{n,(n+1)/2}$ and $H = J^{m,m/2}$, where n is odd and m is even. We first notice that $|E(I^{n,(n+1)/2})| = ½(6n^2 + 5n + 1)$ and $|E(J^{m,m/2})| = ½(6m^2 + 5m - 4)$. We compute PI indices of these graphs. To do this, we have:

$$PI(I^{n,(n+1)/2}) = | E(I^{n,(n+1)/2})|^2 - \Sigma_{e\in E(G)}N(e)$$
$$= (1/4)(6n^2 + 5n + 1)^2 - (1/6)(16n^3+24n^2+23n+9)$$
$$= (1/12)(108n^4 + 148n^3 + 63n^2 - 16n - 15),$$
$$PI(J^{m,m/2}) = | E(J^{m,m/2})|^2 - \Sigma_{e\in E(H)}N(e)$$
$$= (1/4)(6m^2+5m-4)^2 - (1/6)(16m^3+24m^2+11m-12)$$
$$= (1/12)(108m^4+148m^3-117m^2-142m+72).$$

Next we compute the Szeged index of these graphs. To do this, we calculate that $|V(I^{n,(n+1)/2})| = 2n^2 + 3n + 1$ and $|V(J^{m,m/2})| = 2m^2 + 3m - 1$. Consider the graph $G = I^{n,(n+1)/2}$. This graph has two types of vertical edges, say I and II, the rows containing n+1 or n hexagons, respectively. There are also two types of oblique edges, III and IV, those with n + 1 parallel edges and others. Let us define $Sz_1 = \Sigma_{e=uv\in I} N_u(e|G)N_v(e|G)$, $Sz_2 = \Sigma_{e=uv\in II} N_u(e|G)N_v(e|G)$, $Sz_3 = \Sigma_{e=uv\in III} N_u(e|G)N_v(e|G)$, $Sz_4 = \Sigma_{e=uv\in IV} N_u(e|G)N_v(e|G)$. We calculate:

$$Sz_1 = (n+1)\sum_{i=0}^{(n-1)/2}[2n+1+4ni+2i][2n^2+3n+1-2n-1-4ni-2i]$$
$$= 1/3n^6 + 5/3n^5 + 49/12n^4 + 17/3n^3 + 13/3n^2 + 5/3n + 1/4,$$
$$Sz_2 = n\sum_{i=0}^{(n-3)/2}[4n+2+4ni+2i][2n^2+3n+1-4n-2-4ni-2i]$$
$$= 1/3n^6 + 4/3n^5 + 3/4n^4 - 13/12n^3 - 13/12n^2 - 1/4n,$$
$$Sz_3 = \sum_{i=1}^{(n+1)/2} 2iS_i(2n^2+3n+1-S_i)$$
$$= 5/48n^6+253/240n^5+373/96n^4+155/24n^3+59/12n^2+119/80n + 3/32,$$
$$Sz_4 = (n+1)\sum_{i=1}^{(n-3)/2}[S_{(n+1)/2}+2ni+2i][2n^2+3n+1-S_{(n+1)/2}-2ni-2i]$$
$$= 11/24n^6 + 3/4n^5 - 17/6n^4 - 49/6n^3 - 55/8n^2 - 19/12n + 1/4,$$

where $S_i = \sum_{n=1}^{i}(4n-1) = 2i^2 + i$. Then Sz(G) = $Sz_1 + Sz_2 + 4Sz_3 + 2Sz_4$. Using a tedious calculation, we can see that Sz(G) = $2n^6 + 523/60n^5 + 353/24n^4 + 169/12n^3 + 55/6n^2 + 21/5n + 9/8$.

We now consider the graph H = $J^{m,m/2}$ to compute its Szeged index. In this case we have five types of edges. Using a similar argument as above, we conclude that

$$Sz(H) = 2m^6 + 523/60m^5 + 109/12m^4 - 1/2m^3 - 25/12m^2 + 1/30m.$$

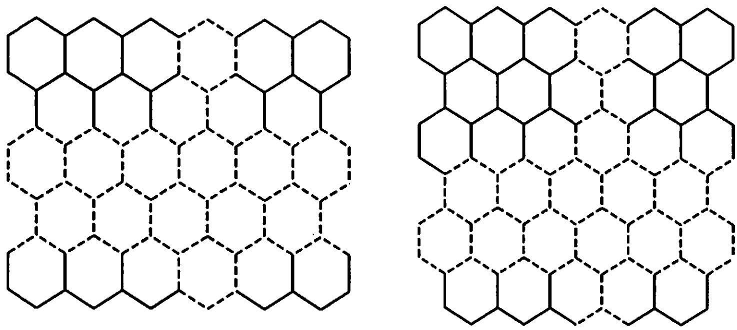
Example 5. Consider the benzenoid graph U(n) of Figure 6, to compute its Szeged and PI indices. This graph has exactly $2n^2 + 4n$ vertices and $3n^2 + 4n - 1$ edges. The graph U(n) has three types of edges, I, II and III. The type I edges of U(n) are vertical, Figure 6(c). Types II and III are those edges marked with heavy and narrow lines in Figure 6(a) and 6(b), respectively. If e is a type I or II edge of U(n) then N(e) = (n+1), but for a type III edge e of U(n), we have $2 \leq N(e) \leq n$. So

$$\sum_{e\in E(U(n))} N(e) = \sum_{e\in I} N(e) + \sum_{e\in II} N(e) + \sum_{e\in III} N(e)$$
$$= 1/3(8n^3 + 18n^2 + 13n - 3).$$

This shows that PI(U(n)) = $(3n^2 + 4n - 1)^2 - 1/3(8n^3 + 18n^2 + 13n - 3) = 1/3(27n^4 + 64n^3 + 12n^2 - 37n + 6)$. We now compute the Szeged index of U(n). To do this, we notice that the type II (III) edges are partitioned into classes II(a) and II(b) (III(a) and III(b)). Let us define $Sz_1 = \sum_{e=uv\in I} N_u(e|G)N_v(e|G)$, $Sz_2 = \sum_{e=uv\in III(a)} N_u(e|G)N_v(e|G)$, $Sz_3 = \sum_{e=uv\in II(a)} N_u(e|G)N_v(e|G)$, $Sz_4 = \sum_{e=uv\in III(b)} N_u(e|G)N_v(e|G)$ and $Sz_5 = \sum_{e=uv\in II(b)} N_u(e|G)N_v(e|G)$. Then

$$Sz(U(n)) = \begin{cases} Sz_1 + 2Sz_2 + Sz_3 + 2Sz_4 + Sz_5 & n \equiv 1 \pmod 2 \\ Sz_1 + 2Sz_2 + Sz_3 + 2Sz_4 + 2Sz_5 & n \equiv 0 \pmod 4). \\ Sz_1 + 2Sz_2 + Sz_3 + 2Sz_4 + 2Sz_5 + (n+1)(n^2/2 + n) & n \equiv 2 \pmod 4) \end{cases}$$

Using a tedious calculation, we can see that:



(a) $I^{n,m}$ (b) $J^{n,m}$

Figure 5. Two types of jagged rectangle benzenoid graphs.

$Sz_1 = 2/3n^6 + 4n^5 + 22/3n^4 + 14/3n^3 + n^2 + 1/3n),$

$$Sz_2 = \begin{cases} 5/48n^6 + 89/120n^5 + 47/32n^4 + 13/24n^3 - 7/6n^2 - 77/60n - 13/32 & 2 \nmid n \\ 5/48n^6 + 67/60n^5 + 129/32n^4 + 71/12n^3 + 17/6n^2 - 17/60n & 2 \mid n \end{cases},$$

$$Sz_3 = \begin{cases} 11/24n^6 + 2n^5 + 5/3n^4 - 29/12n^3 - 25/8n^2 + 5/12n + 1 & 2 \nmid n \\ 11/24n^6 + 13/8n^5 - 17/24n^4 - 151/24n^3 - 19/4n^2 - 1/3n & 2 \mid n \end{cases},$$

$$Sz_4 = \begin{cases} 5/48n^6 + 67/60n^5 + 141/32n^4 + 31/4n^3 + 131/24n^2 + 2/15n - 31/32 & 2 \nmid n \\ 5/48n^6 + 89/120n^5 + 59/32n^4 + 15/8n^3 + 17/24n^2 + 2/15n & 2 \mid n \end{cases}$$

$$Sz_5 = \begin{cases} 11/24n^6 + 2n^5 + 5/3n^4 - 29/12n^3 - 25/8n^2 + 5/12n + 1 & 2 \nmid n \\ 11/24n^6 + 19/8n^5 + 97/24n^4 + 59/24n^3 + 1/2n^2 + 1/6n & 2 \mid n \end{cases}$$

Therefore,

$$Sz(U(n)) = \begin{cases} 2n^6 + 703/60n^5 + 269/12n^4 + 197/12n^3 + 10/3n^2 - 17/15n - 3/4 & 2 \nmid n \\ 2n^6 + 703/60n^5 + 269/12n^4 + 203/12n^3 + 16/3n^2 + 13/15n & 4 \mid n \\ 2n^6 + 703/60n^5 + 269/12n^4 + 197/12n^3 + 23/6n^2 - 2/15n & 2 \nmid n/2 \end{cases}$$

In the Examples 1-4, the PI indices of investigated benzenoid graphs are strictly less than their Szeged indices. We end this paper with the following open question:

Question 2. Let G be a benzenoid graph. Is it true that $PI(G) < Sz(G)$?

A graph is called chordal if each of its cycles of four or more nodes has a chord, which is an edge joining two nodes that are not adjacent in the cycle. An equivalent definition is that induced subgraphs which are simple cycles have at most three nodes. Chordal graphs are a subset of the perfect graphs. It is easy to see that $PI(O_8) = 72$ and $Sz(O_8)$

= 48, where O_8 is octahedral graph. Our calculation on the graphs with the small number of vertices pose the following open question:

Question 3. Let G be a chordal graph. Is it true that always Sz(G) < PI(G)?

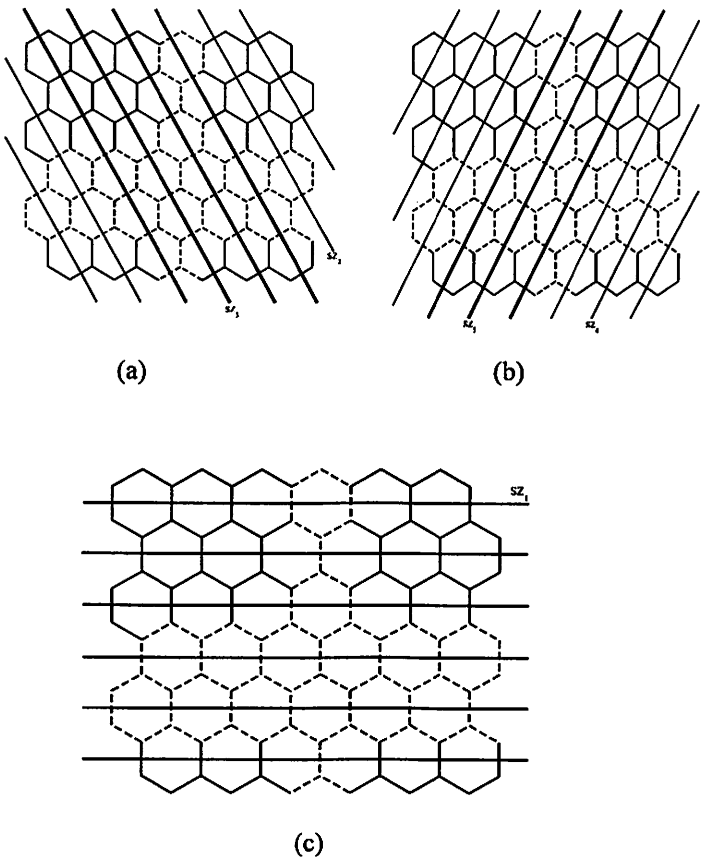


Figure 6. The Benzenoid Graph of U(n) in three shapes.

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