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PI Polynomial of some Benzenoid Graphs

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Abstract

Let G be a connected graph, u; v be vertices of G and e = uv. The number of edges of G lying closer to u than to v is denoted by $n_{eu}(e|G)$ and the number of edges of G lying closer to v than to u is denoted by $n_{ev}(e|G)$. The PI polynomial of G is defined as $PI(G; x) = \sum_{\{u,v\}\subseteq V(G)} x^{N(u,v)}$, where $N(u,v) = n_{eu}(e|G) + n_{ev}(e|G)$, if e = uv; and = 0, otherwise. In this paper, we prove a simple formula which is useful for computing PI polynomial of graphs. Using this formula, the PI polynomial of some important classes of benzenoid graphs, which some of them are related to nanostructures, are computed.

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

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proposed to be used in chemistry. It was introduced in 1947 by Harold Wiener for characterization of alkanes. This index is defined as the sum of all distances between distinct vertices, see [23].

A new topological index introduced very recently by P V. Khadikar, [13-16]. It is defined as the sum of $[n_{eu}(e|G) + n_{ev}(e|G)]$ between all edges e=uv of a graph G, where $n_{eu}(e|G)$ is the number of edges of G lying closer to u than to v and $n_{ev}(e|G)$ 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, [1-6,8,16,19,24,25].

We now describe some notations which will be kept throughout. Benzenoid graphs (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 [16], Khadikar and co-authors critically examined PI index of organic compounds acting as drugs and discussed its applications in Computer-Aided designing of bioactive compounds with special reference to designing of carbonic anhydrase inhibitors, lipophilicity, toxicity, tadpole narcosis, bio-concentration factor, diuretic activity and carcinogenic activity of aromatic hydrocarbons and heterocycles etc. We encourage reader to consult this paper for recent progress in computing PI index of some important classes of chemical compounds and their applications in biochemistry.

Suppose G is a connected graph, u, v are vertices of G and e = uv. In [6], the present authors defined the notion of PI polynomial of a graph as $PI(G;x) = \Sigma_{\{u,v\}\subseteq V(G)} x^{N(u,v)}$, where

$$N(u,v) = \begin{cases} n_{eu}(e\,|\,G) + n_{ev}(e\,|\,G) & uv \in E(G) \\ 0 & uv \notin E(G) \end{cases} .$$

In [20,21] Shiu and co-authors computed the Wiener indices of some important classes of benzenoid graphs. We are very grateful from the referee for pointing out the Wiener indices of these benzenoid graphs and many other benzenoid graphs have also been independently computed by Klavzar, Gutman, Mohar and Rajapakse, [11,17,18]. In this paper the PI polynomial and then PI indices of these graphs are also computed. We only consider connected graphs. Our notation is standard and mainly taken from [7,22].

2. Results and Discussion

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. In this section we calculate the PI polynomial of some benzenoid graphs.

Suppose G is a benzenoid graph and $e \in E(G)$. 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 $PI(G) = |E|^2 - \sum_{e\in E(G)} N(e)$. In [25], we computed the values of N(e) for some classes of benzenoid graphs. We use these values freely throughout the paper. We also prove a formula which is useful in our calculations. Let T be a graph. Then we have:

$$
\begin{aligned}
PI(T;x) &= \sum_{\{u,v\}\subseteq V} x^{N(u,v)} \\
&= \sum_{uv\in E} x^{N(u,v)} + \sum_{uv\notin E} 1 \\
&= \sum_{e=uv\in E} x^{|E|-N(e)} + |E(K_n)| - |E| + |V| \\
&= \sum_{e\in E} x^{|E|-N(e)} + \binom{|V|+1}{2} - |E|.
\end{aligned}
$$

Example 1. Consider the hexagonal triangle graph T(n) of Figure 1, 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, $|E(G)| = 3(2 + 3 + 4 + \ldots + (n + 1)) = 3/2(n^2 + 3n)$ and $|V(G)| = 3 + 5 + \ldots + (2n+1) = n^2 + 4n + 1$.

$$
\begin{aligned}
PI(T(n);x) &= \sum_{\{u,v\}\subseteq V(T(n))} x^{N(u,v)} \\
&= \sum_{e\in E(T(n))} x^{|E(T(n))|-N(e)} + \binom{|V(T(n))|+1}{2} - |E(T(n))| \\
&= 3\sum_{i=2}^{n+1} i x^{3/2(n^2+3n)-i} + \binom{n^2+4n+2}{2} - 3/2(n^2+3n).
\end{aligned}
$$

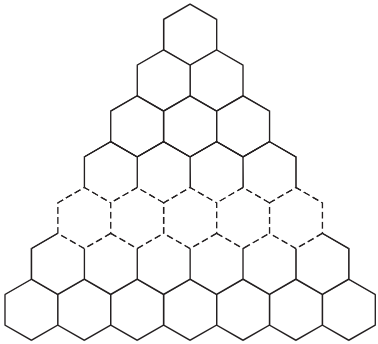


Figure 1. The Hexagonal Triangle Graph T(n)

Example 2. Let H_n be an n-hexagonal net, which is a benzenoid graph consisting of one central hexagon and is surrounded by n – 1 layers of hexagonal cells when $n \geq 1$, Figure 2. 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-hegagonal net. They proved that $W(H_n) = 1/5(164n^5 – 30n^3 + n)$. Here the PI polynomial of this graph is computed. Since the j^{th} row of the graph H_n has exactly k + j vertical edges, $|E(H_n)| = 3\{2[(n+1) + (n+2) + \ldots + (2n - 1)]+ 2n\} = 9n^2 - 3n$. A similar calculation shows that $|V(G)| = 6n^2$.

$$
\begin{aligned}
PI(H_n;x) &= \sum_{\{u,v\}\subseteq V(H_n)} x^{N(u,v)} \\
&= \sum_{e\in E(H_n)} x^{|E(H_n)|-N(e)} + \binom{|V(H_n)|+1}{2} - |E(H_n)| \\
&= 3(2\sum_{i=1}^{n-1}(n+i)x^{9n^2-3n-(n+i)} + 2nx^{9n^2-5n}) + \binom{6n^2+1}{2} - 9n^2 + 3n.
\end{aligned}
$$

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 3. Consider a hexagonal parallelogram $Q_{n,m}$

to compute its PI polynomial. It is clear that $|E(Q_{n,m})|$ = 3mn+2m+2n-1 and $|V(Q_{n,m})| = 2(mn + n + m)$.

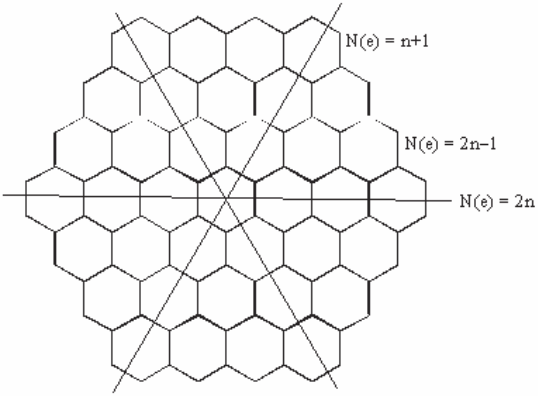


Figure 2. A 4-hexagonal net (circum-circumcoronene).

Without loss of generality, we can assume that m ≤ n. It is easy to see that every edge of $Q_{n,m}$ is vertical, left oblique and right oblique, Figure 3. If e is vertical then N(e) = n + 1 and if e is left oblique then we can consider e as the vertical edge of $Q_{m,n}$ and so N(e) = m + 1. Finally, in the case that e is a right oblique, there are n–m+1 right oblique chains of hexagons (each of which has m hexagons). So by our formula, we have:

$$
\begin{aligned}
PI(Q_{n,m};x) &= \sum\nolimits_{\{u,v\}\subseteq V(Q_{n,m})} x^{N(u,v)} \\
&= \sum\nolimits_{e\in E(Q_{n,m})} x^{|E(Q_{n,m})|-N(e)} + \binom{|V(Q_{n,m})|+1}{2} - |E(Q_{n,m})| \\
&= m(n+1)x^{3mn+2m+n-2} + (nm+2n-m+1)x^{3mn+m+2n-2} - 3mn - 2m \\
&\quad - 2n + 1 + \binom{2(mn+n+m)+1}{2} + 2\sum_{i=1}^{m-1}(i+1)x^{3mn+2m+2n-(i+2)}
\end{aligned}
$$

In [6], we proved that for every graph G, PI′(G;1) = PI(G). Using this result, we have:

$$
PI(Q_{n,m}) = \begin{cases} 9m^2n^2 + 12m^2n + 11mn^2 - 2mn - 5/3m^3 + 4m^2 - 16/3m + 4n^2 - 5n + 3 & n < m \\ 9m^2n^2 + 10m^2n + 11mn^2 - 4mn + 1/3m^3 + 4m^2 - 19/3m + 4n^2 - 6n + 2 & n \ge m \end{cases}
$$

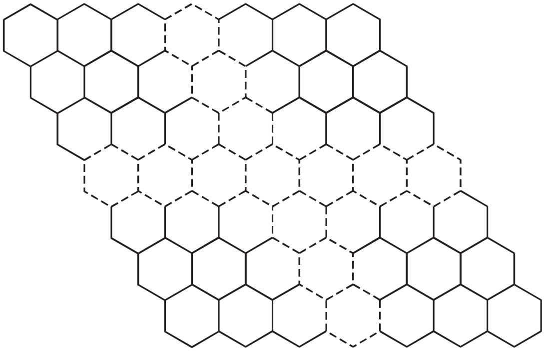


Figure 3. The Hexagonal Parallelogram $Q_{n,m}$.

Example 4. Following Shiu, Tong and Lam [21], 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. The exact expression for the Wiener index of an arbitrary HJR is lengthy to be included here. In what follows, we compute the PI index and then the PI polynomials of $I^{n,m}$, $J^{n,m}$ and $K^{n,m}$. In [6], we proved that for every graph G, $PI'(G;1) = PI(G)$ and so it is enough to compute the PI polynomial of these graphs. We first compute the value of N(e) in these graphs. To do this, we notice that $|E(I^{n,m})| = 6mn + m - n$, $|V(I^{n,m})| = 2m(2n+1)$, $|E(J^{n,m})| = 6mn + m + 2n - 2$, $|V(J^{n,m})| = 4mn + 2m + 2n - 1$, $|E(K^{n,m})| = 6mn + 7m - n - 6$ and $|V(K^{n,m})| = 4mn + 6m - 4$.

Consider the graph $I^{n,m}$ and its arbitrary edge e. To compute N(e), we consider two cases that e is vertical or oblique. Suppose A and B are sets of all vertical edges lie in the long and small rows of this graph, respectively (Figure 4(a)). Then we have:

$$N(e) = \begin{cases} n+1 & e \in A \\ n & e \in B \end{cases}.$$

Suppose e is an oblique edge in the right i^{th} oblique row, Figure 4(a). We consider two cases that $n < m$ and $n \geq m$. If $n < m$ then $N(e) = 2i$ and if $n \geq m$ then we have $N(e) = \begin{cases} 2i & 1 \leq i < m \\ m & m \leq i \leq n \end{cases}$. If e is an oblique edge in the left i^{th} oblique row then by symmetry we find the same formulae for N(e).

$$PI(I^{n,m};x) = \sum_{\{u,v\} \subseteq V(I^{n,m})} x^{N(u,v)}$$

$$= \sum_{e \in E(I^{n,m})} x^{|E(I^{n,m})|-N(e)} + \binom{|V(I^{n,m})|+1}{2} - |E(I^{n,m})|$$

$$= m(n+1)x^{6mn+m-2n-1} + (m-1)nx^{6mn+m-2n} + \binom{4mn+2m+1}{2}$$

$$-(6mn+m-n) + \begin{cases} 4\sum_{i=1}^{m-1} 2ix^{6mn+m-n-2i} + 8m^2(n-m+1)x^{6mn-m-n} & n \geq m \\ 4\sum_{i=1}^{m-1} 2ix^{6mn+m-n-2i} & n < m \end{cases}.$$

Since $PI(I^{n,m}) = PI'(I^{n,m},1)$, we have:

$$PI(I^{n,m}) = \begin{cases} 36m^2n^2 + 4m^2n - 14mn^2 - 4mn + 8/3m^3 + m^2 - 11/3m + 2n^2 & n \geq m \\ 36m^2n^2 + 12m^2n - 14mn^2 - 4mn - 16/3m^3 + 9m^2 - 11/3m + 2n^2 & n < m \end{cases}$$

We now consider the graph $J^{n,m}$ to compute its PI polynomial and PI index. Suppose A_1 and B_1 are the set of all vertical edges lie in the long and small rows of this graph, respectively (Figure 4(b)). Then we have:

$$N(e) = \begin{cases} n+1 & e \in A_1 \\ n & e \in B_1 \end{cases}.$$

Using a similar argument on oblique edges, we have:

$$PI(J^{n,m};x) = \sum_{\{u,v\} \subseteq V(J^{n,m})} x^{N(u,v)}$$

$$= \sum_{e \in E(J^{n,m})} x^{|E(J^{n,m})|-N(e)} + \binom{|V(J^{n,m})|+1}{2} - |E(J^{n,m})|$$

$$= m(n+1)x^{6mn+m+n-3} + mnx^{6mn+n+m-2} + \binom{4mn+2m+2n}{2} - (6mn+2n+m-2) +$$

$$+ \begin{cases} 2\sum_{i=1}^{m}(2i)x^{6mn+2n+m-2-2i} + 2\sum_{i=2}^{m}(2i-1)x^{6mn+2n+m-1-2i} + 2(n-m)(2m+1)x^{6mn+2n-m-3} & n > m \\ 2\sum_{i=1}^{m}(2i)x^{6mn+2n+m-2-2i} + 2\sum_{i=2}^{m}(2i-1)x^{6mn+2n+m-1-2i} & n \leq m \end{cases}$$

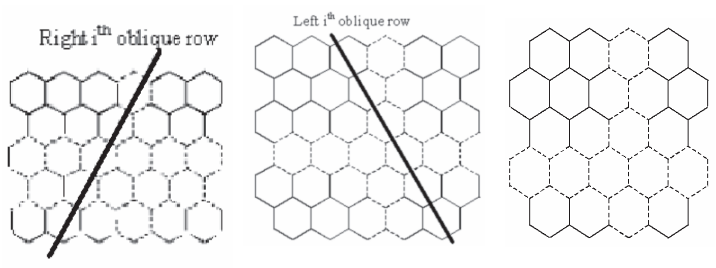
Therefore,

$$PI(J^{n,m}) = \begin{cases} 36m^2n^2 + 4m^2n + 22mn^2 - 30mn + 8/3m^3 + 5m^2 - 11/3m + 4n^2 - 10n + 6 & n > m \\ 36m^2n^2 + 12m^2n + 22mn^2 - 22mn - 16/3m^3 - 3m^2 - 17/3m + 4n^2 - 8n + 6 & n \le m \end{cases}$$

Finally, we compute the PI polynomial and PI index of the graph $K^{n,m}$. Using a similar argument as above, we have:

$$\begin{aligned} PI(K^{n,m};x) &= \sum_{\{u,v\} \subseteq V(K^{n,m})} x^{N(u,v)} \\ &= \sum_{e \in E(K^{n,m})} x^{|E(K^{n,m})| - N(e)} + \binom{|V(K^{n,m})|+1}{2} - |E(K^{n,m})| \\ &= m(n+1)x^{6mn+7m-2n-7} + (m-1)(n+2)x^{6mn+7m-2n-8} + \binom{4mn+6m-3}{2} - (6mn+7m-n-6) \\ &+ \begin{cases} 4\sum_{i=1}^{m}(2i-1)x^{6mn+7m-n-5-2i} & n < m \\ 4\sum_{i=1}^{m}(2i-1)x^{6mn+7m-n-5-2i} + 4m(n-m+1)x^{6mn+5m-n-6} & n \ge m \end{cases} \end{aligned}$$

$$PI(K^{n,m}) = \begin{cases} 36m^2n^2 + 84m^2n - 14mn^2 - 92mn + 16/3m^3 + 49m^2 - 271/3m + 2n^2 + 16n + 36 & n < m \\ 36m^2n^2 + 88m^2n - 14mn^2 - 92mn + 4/3m^3 + 53m^2 - 271/3m + 2n^2 + 16n + 36 & n \ge m \end{cases}$$



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

Figure 4. Two types of benzenoid graphs introduced by Shiu et al [20].

Example 5. Consider the benzenoid graph U(n,m) consisting of m chains of n-hexagons, Figure 5. This graph has exactly 2(mn+m+n) vertices and 3mn + 2m+ 2n – 1 edges. If e is a vertical edge then N(e) = n+1. Suppose e is a right oblique edge in the i^{th} row. Our main proof will consider two cases:

Case 1. $[m/2] \le n$. In this case we have:

$$N(e)=\begin{cases}2i & 1\le i\le [m/2]\\ m+1 & [m/2]<i\le n\end{cases},$$

where [x] denotes the greatest integer ≤ x. Therefore,

$$\begin{aligned}PI(U(n,m);x) &= \sum_{\{u,v\}\subseteq V(U(n,m))} x^{N(u,v)}\\ &= \sum_{e\in E(U(n,m))} x^{|E(U(n,m))|-N(e)} + \binom{|V(U(n,m))|+1}{2} - |E(U(n,m))|\\ &= 2\sum_{i=1}^{[m/2]} 2ix^{3mn+2m+2n-1-2i} + 2\sum_{i=1}^{[m/2]-1}(2i+1)x^{3mn+2m+2n-2-2i}\\ &\quad + m(n+1)x^{3mn+2m+n-2} - (3mn+2m+2n-1)\\ &\quad + 2(n-[m/2])(m+1)x^{3mn+m+2n-2} + \binom{2(mn+m+n)+1}{2}.\end{aligned}$$

Case 2. [m/2] > n. In this case we consider two separate cases that m is odd or even. If m is even and e is an edge of right i^{th} oblique row then N(e) = 2i, 1 ≤ i ≤ n and if e is left i^{th} oblique row then N(e) = 2i + 1, 1 ≤ i ≤ n–1. Therefore by symmetry of the graph, we have:

$$\begin{aligned}PI(U(n,m);x) &= \sum_{\{u,v\}\subseteq V(U(n,m))} x^{N(u,v)}\\ &= \sum_{e\in E(U(n,m))} x^{|E(U(n,m))|-N(e)} + \binom{|V(U(n,m))|+1}{2} - |E(U(n,m))|\\ &= 2\sum_{i=1}^{n} 2ix^{3mn+2m+2n-1-2i} + 2\sum_{i=1}^{n-1}(2i+1)x^{3mn+2m+2n-2-2i}\\ &\quad + m(n+1)x^{3mn+2m+n-2} - (3mn+2m+2n-1)\\ &\quad + 2(m/2-n)(2n+1)x^{3mn+2n-2} + \binom{2(mn+m+n)+1}{2}.\end{aligned}$$

If m is odd, a similar argument shows:

$$\begin{aligned}PI(U(n,m);x) &= \sum_{\{u,v\}\subseteq V(U(n,m))} x^{N(u,v)}\\ &= \sum_{e\in E(U(n,m))} x^{|E(U(n,m))|-N(e)} + \binom{|V(U(n,m))|+1}{2} - |E(U(n,m))|\\ &= 2\sum_{i=1}^{n} 2ix^{3mn+2m+2n-1-2i} + 2\sum_{i=1}^{n-1}(2i+1)x^{3mn+2m+2n-2-2i}\\ &\quad + m(n+1)x^{3mn+2m+n-2} - (3mn+2m+2n-1)\\ &\quad + 2([m/2]-n+1)(2n+1)x^{3mn+2n-2} + \binom{2(mn+m+n)+1}{2}.\end{aligned}$$

Finally, using equation PI(G) = PI′(G;1), one can calculate the PI index of the graph U(n,m).

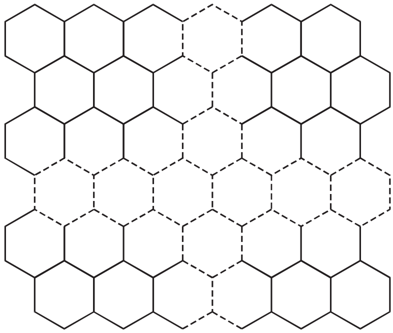


Figure 5. The Benzenoid Graph of U(n,m).

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