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Computing a Counting polynomial of an infinite family of linear polycene parallelogram benzenoid graph *P(a,b)*

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ABSTRACT

Omega polynomial was defined by *M.V. Diudea* in 2006 as $\Omega(G,x)=\sum_{e\in E(G)} x^{n(e)}$ where the number of edges co-distant with *e* is denoted by *n(e).* One can obtain Theta *Θ*, Sadhana *Sd* and Pi *Π* polynomials by replacing $x^{n(e)}$ with $n(e)x^{n(e)}$, $x^{|E|-n(e)}$ and $n(e)x^{|E|-n(e)}$ in Omega polynomial, respectively. Then Theta *Θ*, Sadhana *Sd* and Pi *Π* indices will be the first derivative of *Θ*(x), *Sd(x)* and *Π*(x) evaluated at *x=1*. In this paper, Pi *Π*(G,x) polynomial and Pi *Π*(G) index of an infinite family of linear polycene parallelogram benzenoid graph *P(a,b)* are computed for the first time.

Indexing terms/Keywords

Molecular graph; benzenoid graph; linear polycene parallelogram; Omega polynomial; Pi *Π*(G,x) polynomial*;* Pi *Π*(G) index*; qoc strip*

SUBJECT CLASSIFICATION

E.g., Mathematics Subject Classification; 05C05, 05C12

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INTRODUCTION

Let *G=(V,E)* be a connected bipartite graph with the vertex set *V=V(G)* and the edge set *E=E(G),* without loops and multiple edges. Suppose *n, e* and *h* be the number of carbon vertices/atoms, edges/bonds between them and hexagons, in a molecular graph *G*.

In graph theory, a topological index is a real number related to a molecular graph, which is a graph invariant. There are several topological indices already defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of the molecules. The oldest topological index is Wiener index which was introduced by Chemist *Harold Wiener* [1]. The *Wiener index* [1] is defined as

$$W(G)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)} d(u,v)$$

The distance *d(u,v)* between *u* and *v* is defined as the length of a minimum path between *u* and *v*. Two edges *e=uv* and *f=xy* of *G* are called co-distant, "*e co f*", if and only if *d(u,x)=d(v,y)=k* and *d(u,y)=d(v,x)=k+1* or vice versa, for a non-negative integer *k*. It is easy to see that the relation "co" is reflexive and symmetric but it is not necessary to be transitive. The Omega polynomial *Ω(G,x)* has been defined by *M.V. Diudea* as follows [2-5]:

$$\Omega(G,x)=\sum_{e\in E(G)} \mathrm{x}^{n(e)}$$

where, *n(e)* denotes the number of edges co–distant with the edge *e*. It is easy to see that the Omega polynomial *Ω(G,x)* counts equidistant edges in graph *G*.

Sadhana index *Sd(G)* for counting qoc strips in *G* was defined by *P.V. Khadikar et al.* [6,7] as

$$Sd(G)=\sum_{e\in E(G)}\left(|E(G)|-n(e)\right)$$

Also, Sadhana polynomial of a graph *G* as defined by *A.R. Ashrafi et al.* [8] as

$$Sd(G,x)=\sum_{e\in E(G)} \mathrm{x}^{|E(G)|-n(e)}$$

Recently, Thete *Θ(G,x)* and Pi *Π(G,x)* polynomials for counting qoc strips in *G* were defined by *Diudea* as

$$\Theta(G,x)=\sum_{e\in E(G)} n(e)\mathrm{x}^{n(e)}$$

$$\Pi(G,x)=\sum_{e\in E(G)} n(e)\mathrm{x}^{|E(G)|-n(e)}$$

By definition of Omega polynomial, one can obtain Theta *Θ*, Sadhana *Sd* and Pi *Π* polynomials by replacing $x^{n(e)}$ with $n(e)x^{n(e)}$, $x^{|E|-n(e)}$ *and* $n(e)x^{|E|-n(e)}$ in Omega polynomial, respectively. Theta *Θ*, Sadhana *Sd* and Pi *Π* indices will be the first derivative of *Θ*(x), Sd(x) and *Π*(x) evaluated at *x=1*.

Also, first derivative of omega polynomial (in *x=1*), equals the number of edges in the graph *G*.

$$\Omega'(G,x)=\sum_{e\in E(G)} n(e)=|E(G)|$$

Throughout this paper, our notation is standard and taken from the standard book of graph theory [1, 9, 10] and for more study about Omega polynomial and other counting polynomilas see paper serices [11-39].

In this paper, Pi *Π*(G,x) polynomial and Pi *Π*(G) index of an infinite family of linear polycene parallelogram benzenoid graph *P(a,b)* are computed for the first time. We encourage the reader to consult papers [33-35, 40-42] and see general representation of this family of benzenoid graph in Figure1.

Main Results and Discussions

In this section by using definition of Pi *Π*(G,x) polynomial and Pi *Π*(G) index, we compute these counting polynomial and its index for of an infinite family of linear polycene parallelogram benzenoid graph *P(a,b).*

A general representation of linear polycene parallelogram benzenoid graph *P(a,b)* depicted in Figure 1, with *2ab+2a+2b* vertices/atoms (|*V(P(a,b))*|) and *3ab+2a+2b*-1 edges/bonds (|*E(P(a,b))*|). For further study and more detail of this family of benzenoid graph readers can see references [33-35, 40-42].

An especial case of this family is symetric linear parallelogram benzenoid *P(a,a)*. It is easy to see that *P(a,a)* $\forall a\in\mathbb{N}$. has *2a(a+2)* vertices and $\frac{3}{2}$ *a(a+3)* $3a^2+4a-1$ edges. Now, By these terminologies, we will have the following theorem for Pi *Π*(G,x) polynomial and Pi *Π*(G) index of linear parallelogram benzenoid *P(a,b)* $\forall a,b\in\mathbb{N}$.

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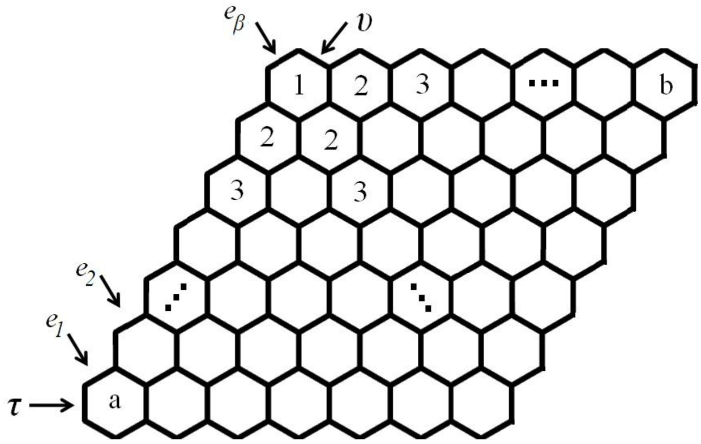

Fig. 1. A 2-D graph of of linear polycene parallelogram benzenoid graph *P(a,b)*.

Theorem 1. Consider linear polycene parallelogram benzenoid graph *P(a,b)* $\forall a,b\in\mathbb{N}-\{1\}$. and $Max\{a,b\}=\alpha$ & $Min\{a,b\}=\beta$ (see Fig. 1). Then

$$\Pi(P(\alpha,\beta),x)=(\alpha\beta+\alpha-\beta^2+1)x^{3\alpha\beta+2\alpha+3\beta-2}+2\sum_{j=2}^{\beta} jx^{3\alpha\beta+2\alpha+2\beta-2-j}+\beta(\alpha+1)x3\alpha\beta-\beta-2+\alpha(\beta+1)x3\alpha\beta-\alpha-2$$

$$\Pi(P(\alpha,\beta))=9\alpha^2\beta^{2+}8\alpha^2\beta+7\alpha\beta^2-\tfrac{1}{3}\beta^3-10\alpha\beta+4\alpha^2+4\beta^2-6\alpha-\tfrac{19}{3}\beta+2$$

Proof. By Fig. 1, there are three distinct cases of *qoc* strips in linear polycene parallelogram benzenoid graph *P(a,b)*. We denote the corresponding edges by $e_1,\dots, e_\beta, \tau$ and υ. By using Table 1, Fig. 1 and on based the integer numbers *n* and *m*, we have two following computations.

Table 1. The number of co-dstant edges of τ, υ and e_i, $i=1,\dots,\beta$ ($\beta=Min\{a,b\}$).

No	Number of codistant edges	Type of Edges
a+1	*b*	υ
b+1	*a*	τ
i+1	*2*	e_i *(i=1,…,β-1)*
β+1	*|a-b|+1*	e_β

I. $\forall a\geq b\in\mathbb{N}-\{1\}$ & $|E(P(a,b))|=3ab+2a+2b-1$, then

$$\Pi(P(a,b),x)=\sum_{e\in E\left(P(a,b)\right)} n(e)x^{|E(P(a,b))|-n(e)}$$

$$=(|a-b|+1)\times(b+1)x^{|E|-b-1}+2\times\sum_{i=1}^{b-1}(i+1)x^{|E|-i-1}+b\times(a+1)x^{|E|-a-1+}a\times(b+1)x^{|E|-b-1}$$

Thus,

$$\Pi(P(a,b))=\Pi'(G_n,x)|_{x=1}=\frac{\partial\left((a-b+1)(b+1)x^{|E|-b-1}+2\sum_{j=2}^{b} ix^{|E|-j}+b(a+1)x^{|E|-a-1}+a(b+1)x^{|E|-b-1}\right)}{\partial x}|_{x=1}$$

$$=9a^2b^{2+}8a^2b+7ab^2-\tfrac{1}{3}b^3-10ab+4a^2+4b^2-6a-\tfrac{19}{3}b+2$$

II. $\forall b<a\in\mathbb{N}-\{1\}$ & $|E(P(a,b))|=3ab+2a+2b-1$, then

$$\Pi(P(a,b),x)=(|a-b|+1)\times(a+1)x^{|E|-a-1}+2\times\sum_{j=1}^{a-1}(j+1)x^{|E|-(j+1)}+b\times(a+1)x^{|E|-a-1+}a\times(b+1)x^{|E|-b-1}$$

And similarly, $\Pi(P(a,b))=9a^2b^{2+}7a^2b+8ab^2-\tfrac{1}{3}a^3-10ab+4a^2+4b^2-\tfrac{19}{3}a-6b+2$

Now, these complete the proof of Theorem 1.■

Theorem 2. Pi polynomial and Pi index of symetric linear polycene parallelogram *P(γ,γ)*, for *γ>1* are equal to

- $\Pi(P(\gamma,\gamma),x)=2\gamma(2\gamma+1)x^{3\gamma^2+2\gamma-2}+(\gamma+1)x^{3\gamma^2+5\gamma-2}+2\sum_{j=2}^{\gamma} jx^{3\gamma^2+4\gamma-2-j}$
- $\Pi(P(\gamma,\gamma))=9\gamma^{4}+\frac{44}{3}\gamma^{3}-\frac{37}{3}\gamma+2$

Proof. By considering *Max{a,b}=Min{a,b}=γ* (see Fig. 1), the proof is analogous to the proof of Theorem 1.

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