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Research article

Π(G,X) Polynomial and Π(G) Index of V-phenylenic Planar, Nanotubes and Nanotori

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Abstract

In this paper, we study some properties of a new counting polynomial of (molecular) graphs that called Pi Π(G,x) polynomial. This counting polynomial and its index were proposed by M.V. Diudea. It is defined on the ground of "opposite edge strips" ops and Pi Π(G,x)= polynomial can also be calculated by ops "opposite edge strips" counting. In continue, closed analytical formulas for Π(G,x) and Π(G) of a physico chemical structure of V-phenylenic Planar VPHP[m,n], Nanotubes VPHX[m,n] and Nanotori VPHY[m,n] are given.

Keywords: Molecular graph, V-phenylenic Nanotubes and Nanotori, Counting polynomial, Pi Π(G,x) polynomial, qoc strip.

1. INTRODUCTION

Let *G=(V;E)* be a simple molecular graph without directed and multiple edges and without loops, the vertex and edge sets of it are represented by *V=V(G)* and *E=E(G),* respectively. In chemical graph theory and in mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. In other words, the vertices correspond to the atoms of the molecule, and the edges represent to the chemical bonds. Also, if *e* is an edge of *G*, connecting the vertices *u* and *v*, then we write *e=uv* and say "*u* and *v* are adjacent".
Chemical graph theory is a branch of mathematical chemistry which applies graph theory to mathematical modeling of chemical phenomena [1-3]. This theory had an important effect on the development of the chemical sciences. Mathematical chemistry is a branch of theoretical chemistry for discussion and prediction of the molecular structure using mathematical methods without necessarily referring to quantum mechanics.

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Two edges/bonds *e=uv* and *f=xy* of *G* are called co-distant, "*e* co *f*", if and only if they obey the following relation: [4, 5]

$$d(v,x)=d(v,y)+1=d(u,x)+1=d(u,y)$$

Relation *co* is reflexive, that is, *e co e* holds for any edge *e* of *G*; it is also symmetric, if *e co f* then *f co e* and in general, relation *co* is not transitive. If "*co*" is also transitive, thus an equivalence relation, then *G* is called a *co-graph* and the set of edges is $C(e):=\{f\in E(G)|\ e\ co\ f\}$), called an *orthogonal cut* (denoted by *oc*) of *G*. *Klavžar* [6] has shown that relation *co* is a theta *Djoković* [7], and *Winkler* [8] relation.
In other words, let *m(G,c)* be the number of qoc strips of length *c* (i.e., the number of cut-off edges) in the graph *G*. The *Omega Polynomial Ω(G,x),* [9-12] for counting *qoc* strips in *G* was defined by *Diudea* as

$$\Omega(G,x)=\sum_{c} m(G,c)\mathrm{x}^{c}$$

The summation runs up to the maximum length of *qoc* strips in *G*. The first derivative (in *x*=1) equals the number of edges in the graph

$$\Omega'(G,1)=\sum\nolimits_{c} m(G,c)\times c=\left|E(G)\right|$$

Other counting polynomials "*Θ(G,x), Sd(G,x)* and *Π(G,x)*" was defined as

$$\Theta(G,x)=\sum_{c} m(G,c)c.\mathrm{x}^{c}$$

$$Sd(G,x)=\sum_{c} m(G,c)\mathrm{x}^{|E(G)|-c}$$

$$\Pi(G,x)=\sum_{c} m(G,c)c.\mathrm{x}^{|E(G)|-c}$$

The first derivative (computed at *x=1*) of these counting polynomials provide interesting topological indices [13-24]:

$$\Theta'(G,1)=\sum\nolimits_{c} m(G,c)\times c^{2}$$

$$Sd'(G,1)=\sum\nolimits_{c} m(G,c)\times(\left|E(G)\right|-c)$$

$$\Pi'(G,1)=\sum\nolimits_{c} m(G,c)\times c(\left|E(G)\right|-c)$$

In Refs [25-44] some topological indices of a physico chemical structure of V-phenylenic nanotube and V-phenylenic nanotori are computed. In addition, the *Sadhana Polynomial* and *index* of V-phenylenic nanotube and nanotori *Sd(G,x)* were computed in 2008 by *A.R. Ashrafi et. al*, [24] and also, the *Theta Polynomial* and *index* of V-phenylenic planar, nanotube and nanotori were computed recently by *M.R. Farahani* [23]. In this report, we continue this work to compute a closed formula for *Π(G,x)* and *Π(G)* of molecular graphs V-phenylenic Planar *VPHP[m,n]*, Nanotubes *VPHX[m,n]* and Nanotori *VPHY[m,n]*. Our notation is standard and mainly taken from Refs [1-5].

2. Main Results and Discussion

The goal of this section is to computing the Pi polynomial *Π(G,x)* and index *Π(G)* of molecular graphs V-phenylenic Planar, nanotube and nanotori. The novel phenylenic and naphthylenic lattices proposed can be constructed from a square net embedded on the toroidal surface. Phenylenes are polycyclic conjugated molecules, composed of four membered ring (=square) and six-membered rings (=hexagons) such that every four membered ring 4-membered cycle is adjacent to two 6-membered cycles, and no two six-membered rings are mutually adjacent. Each four-membered ring lies between two six-membered rings, and each hexagon is adjacent only to four-membered rings [25-30].

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Following *M.V. Diudea* [31] for all integer number *m,n*, we denote a V-Phenylenic nanotube and V-Phenylenic nanotorus by *G=VPHX[m,n]* and *H=VPHY[m,n]*, respectively. It is essy to see that all molecular graph V-Phenylenic have *6mn* vertices/atoms and there are *9mn-m* and *9mn* edges/bonds in *VPHX[m,n]* and *VPHY[m,n]*, respectively. And also we denote a V-Phenylenic planar with *6mn* vertices/atoms and *9mn-2n-m* edges/bonds by *K=VPHP[m,n]*. A general representation of these molecular graphs and nano structures are shown in Figure 1, Figure 2 and Figure 3 and paper series [25-44].
Now by using *Cut Method* and Orthogonal Cut *Method*, we have Theorems 1, 2 and 3 for Pi *Π(G,x)* polynomial and *Π(G)* index of three molecular graphs V-phenylenic Planar *VPHP[m,n]*, Nanotubes *VPHX[m,n]* and Nanotori *VPHY[m,n]* as follow.

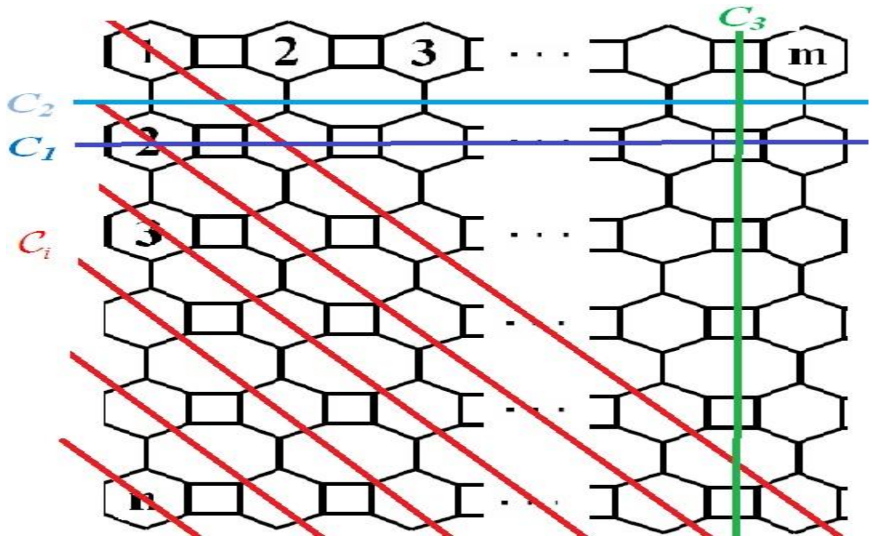

Figure 1: [23] The 2-D of V-Phenylenic Nanotube K=*VPHP[m,n]*.

Theorem 1. $\forall m,n \in \mathbb{N}$, Consider the V-Phenylenic Planar *K=VPHP[m,n]* then the Pi polynomial of *VPHP[m,n]* is:

$\forall\ m\geq n,$ $$\Pi(VPHP[m,n],x)=2mnx^{9mn-2n-3m}+2n(3m-2n+1)x^{9mn-4n-m}+8\sum_{i=1}^{n-1} ix^{9mn-2n-m-2i}+m(n-1)x^{9mn-2n-2m}$$

$\forall\ m<n,$ $$\Pi(VPHP[m,n],x)=2n(n-1)x^{9mn-4n-m}+2m(2n-2m+3)\,x^{9mn-2n-3m}+8\sum_{i=1}^{m-1} ix^{9mn-2n-m-2i}+m(n-1)x^{9mn-2n-2m}$$

And the Pi index of *VPHP[m,n]* is

$\forall\ m\geq n,$ $\Pi(VPHP[m,n])=81m^2n^2+\frac{8}{3}n^3-48mn^2-23m^2n+8n^2+2m^2+4mn-\frac{8}{3}n$

$\forall\ m<n,$ $\Pi(VPHP[m,n])=81m^2n^2+\frac{8}{3}m^3-27m^2n-40mn^2-2m^2+8n^2+4mn-\frac{8}{3}n$

Theorem 2. The *Π* polynomial and *Π* index of V-Phenylenic nanotube *VPHX[m,n]* are equal to:

$$\Pi(VPHX[m,n],x)=6mnx^{9mn-2n-m}+m(n-1)x^{9mn-2m}+2mnx^{9mn-3m}$$

$$\Pi(VPHX[m,n])=81m^2n^2-18m^2n-12mn^2$$

Theorem 3. The Π polynomial and Π index of V-Phenylenic Nanotori $H=VPHY[m,n]$ are equal to:

$$\Pi(VPHY[m,n],x)=4mnx^{9mn-2nm}+2mnx^{9mn-2n}+2mnx^{9mn-2m}+m(n-1)x^{9mn-m}$$

$$\Pi(VPHY[m,n])=73m^2n^2-5nm^2-4mn^2+m^2$$

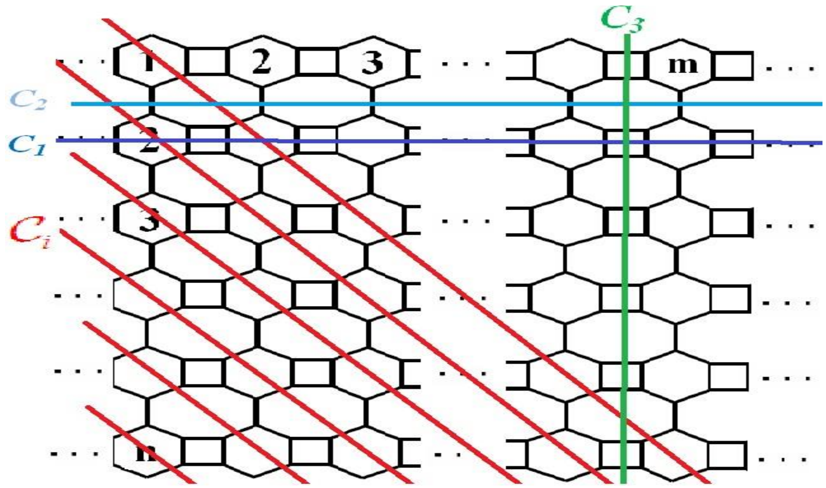

Figure 2: [23] The 2-D of V-Phenylenic Nanotube G=*VPHX[m,n]*.

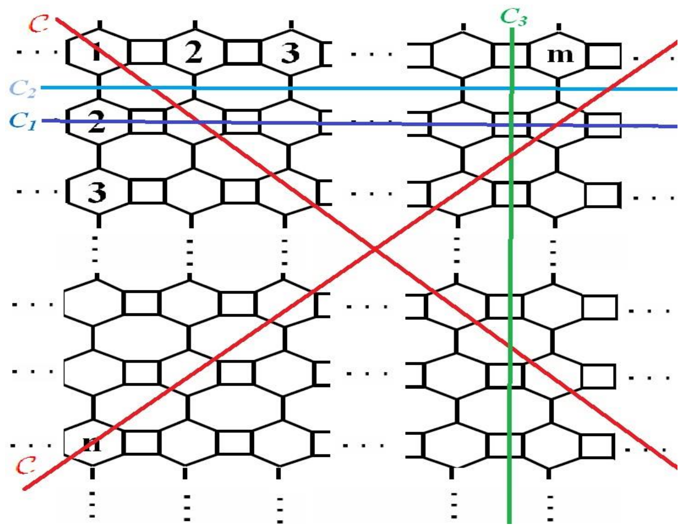

Figure 3: [23] The 2-D of V-Phenylenic Nanotube H=*VPHY[m,n]*.

To compute the Pi polynomial and index of Phenylenic molecular graph, it is enough to calculate $C(e)$ for all edges/bonds. So, by using the Cut Method and from Figures 1 and results herein References 23, 24 one can see that there are four types of edges-cuts for the V-Phenylenic Planar $K=VPHP[m,n]$. We denote the corresponding edges-cut by C_i $(i=1,...\ Max\{m,n\})$ and C_i $(i=1,2,3)$. By definitions of $\Pi(G,x)$, $\Pi(G)$ and Tables 1 and 2, we have

$\forall\ m\geq n:$

$$\Pi(VPHP[m,n],x)=\sum_c m\big(VPHP[m,n],c\big).c.\mathrm{x}^{|E(VPHP[m,n])|-C}$$

$$=2mnx^{9mn-2n-m-2m}+m(n-1)x^{9mn-2n-m-m}+2n(m-1)x^{9mn-2n-m-2n}$$

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$$+4\sum_{i=1}^{n-1}(2i)\,x^{9mn-2n-m-2i} \;+4n(m-n+1)x^{9mn-2n-m-2n}$$

$$=2mnx^{9mn-2n-3m}+2n(3m-2n+1)x^{9mn-4n-m} \;+8\sum_{i=1}^{n-1} ix^{9mn-2n-m-2i}$$

$$+m(n-1)x^{9mn-2n-2m}$$

Table 1: All quasi-orthogonal cuts of V-Phenylenic Planar K=*VPHP[m,n]*, for $m\geq n$.

quasi-orthogonal cuts	The length of qoc strips	The number of qoc strips
C_1	$2m$	n
C_2	m	$n-1$
C_3	$2n$	$m-1$
$C_i\ \forall\ i=1,\dots,n-1$	$2i$	4
C_n	$2n$	$4(m-n+1)$

$$\forall\ m<n:\ \Pi(VPHP[m,n],x)=2mnx^{9mn-2n-m-2m}+m(n-1)x^{9mn-2n-m-m}+2n(m-1)x^{9mn-2n-m-2n}$$

$$+4\sum_{i=1}^{m-1}(2i)\,x^{9mn-2n-m-2i} \;+4m(n-m+1)x^{9mn-2n-m-2m}$$

$$=2n(n-1)x^{9mn-4n-m}+2m(2n-2m+3)\,x^{9mn-2n-3m}$$

$$+8\sum_{i=1}^{m-1} ix^{9mn-2n-m-2i} \;+m(n-1)x^{9mn-2n-2m}$$

Table 2: All quasi-orthogonal cuts of V-Phenylenic Planar K=*VPHP[m,n]*, for $m<n$.

quasi-orthogonal cuts	The length of qoc strips	The number of qoc strips
C_1	$2m$	n
C_2	m	$n-1$
C_3	$2n$	$m-1$
$C_i\ \forall\ i=1,\dots,m-1$	$2i$	4
C_m	$2m$	$4(n-m+1)$

And alternatively, for $m\geq n$:

$$\Pi'\left(VPHP[m,n],x\right)\big|_{x=1}=\left(2mnx^{9mn-2n-3m}+2n(3m-2n+1)x^{9mn-4n-m}+8\sum_{i=1}^{n-1}ix^{9mn-2n-m2i}+m(n-1)x^{9mn-2n-2m}\right)'\Bigg|_{x=1}$$

$$=2mn(9mn-2n-3m)+2n(3m-2n+1)(9mn-4n-m)$$

$$+\sum_{i=1}^{n-1}8i\left(9mn-2n-m-2i\right)+m(n-1)(9mn-2n-2m)$$

$$=81m^2n^2+\tfrac{8}{3}n^3-48mn^2-23m^2n+8n^2+2m^2+4mn-\tfrac{8}{3}n$$

And also, for $m<n$:

$$\Pi(VPHP[m,n]) = \left(2n(n-1)x^{9mn-4n-m} + 2m(2n-2m+3)\,x^{9mn-2n-3m} + 8\sum_{i=1}^{m-1} i x^{9mn-2n-m-2i} + m(n-1)x^{9mn-2n-2m}\right)'\Bigg|_{x=1}$$

$$=2n(n-1)(9mn-4n-m)+2m(2n-2m+3)(9mn-2n-3m)$$

$$+\sum_{i=1}^{m-1} 8i(9mn-2n-m-2i) + m(n-1)(9mn-2n-2m)$$

$$=81m^2n^2+ {}^{8}\!/_{3}\, m^3-27m^2n-40mn^2-2m^2+8n^2+4mn- {}^{8}\!/_{3}\, n$$

From Figures 2, one can see that there are four types of edges-cuts in V-Phenylenic nanotube $G=VPHX[m,n]$ (we denote these edges-cuts by C_i $(i=1,2,3)$ and C, see Table 3).

Table 3: All quasi-orthogonal cuts of V-Phenylenic Nanotube G=$VPHX[m,n]$.

quasi-orthogonal cuts	The length of qoc strips	The number of qoc strips
C_1	2m	n
C_2	m	$n-1$
C_3	2n	m
C	2n	$2m$

Now, since G has $9mn-m$ edges, thus by using Tables 3 and the results from [23, 24], we have

$$\Pi(VPHX[m,n],x) = \sum_c m(VPHX[m,n],c).c.x^{|E(VPHX[m,n])|-C}$$

$$=4mnx^{9mn-m-2n}+2mnx^{9mn-m-2n}+m(n-1)x^{9mn-m-m}+2mnx^{9mn-m-2m}$$

$$=6mnx^{9mn-2n-m}+m(n-1)x^{9mn-2m}+2mnx^{9mn-3m}$$

And alternatively,

$$\Pi(VPHX[m,n]) = \left(6mnx^{9mn-2n-m} + m(n-1)x^{9mn-2m} + 2mnx^{9mn-3m}\right)'\Big|_{x=1}$$

$$=6mn(9mn-2n-m)+m(n-1)(9mn-2m)+2mn(9mn-3m)$$

$$=81m^2n^2-18m^2n-12mn^2$$

In finally, for the V-Phenylenic Nanotori $H=VPHY[m,n]$ with $6mn$ vertices/atoms and $9mn$ edges/bonds for all integer number m,n, Figure 3 and Table 4 imply that the Pi polynomial and Pi index of H are equal to:

$$\Pi(VPHY[m,n],x) = \sum_c m(VPHY[m,n],c).c.x^{|E(VPHY[m,n])|-C}$$

$$=4mnx^{9mn-2nm}+2mnx^{9mn-2n}+2mnx^{9mn-2m}+m(n-1)x^{9mn-m}$$

And alternatively,

$$\Theta(VPHY[m,n]) = \left(4mnx^{9mn-2nm} + 2mnx^{9mn-2n} + 2mnx^{9mn-2m} + m(n-1)x^{9mn-m}\right)'\Big|_{x=1}$$

$$=4mn(9mn-2nm)+2mn(9mn-2n)+2mn(9mn-2m)+m(n-1)(9mn-m)$$

$$=73m^2n^2-5nm^2-4mn^2+m^2$$

Table 4: All quasi-orthogonal cuts of V-Phenylenic Nanotori $H=VPHY[m,n]$ with $9mn$ edges/bonds

quasi-orthogonal cuts	The length of qoc strips	The number of qoc strips
C_1	$2m$	n
C_2	m	$n-1$
C_3	$2n$	m
C	$2nm$	2

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