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Research article

Computing Θ(G,x) Polynomial and Θ(G) Index of V-phenylenic Planar, Nanotubes and Nanotori

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Abstract

A counting polynomial, called Omega *Ω(G,x)*, was proposed by Diudea. It is defined on the ground of "opposite edge strips" ops. Theta $\Theta(G,x)=\sum_{c} m(G,c)c.\mathrm{x}^{c}$ polynomial can also be calculated by ops counting. In this paper we compute this counting polynomial and its index for V-phenylenic Planar, Nanotubes and Nanotori.

Keywords: Omega polynomial, Theta polynomial, qoc strip, V-phenylenic Nanotubes and Nanotori.

Introduction

Mathematical calculations are absolutely necessary to explore important concepts in chemistry. 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. 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. A topological index is a numerical value associated with chemical constitution purporting for correlation of chemical structure properties, chemical reactivity or biological activity.
Let $G(V, E)$ be a connected molecular graph without multiple edges and loops, with the vertex set $V(G)$ and edge set $E(G)$, and vertices/atoms $x, y \in V(G)$. Two edges $e=uv$ and $f=xy$ of G are called codistant (briefly: e co f) if they obey the topologically parallel edges relation. For some edges of a connected graph G there are the following relations satisfied [1-3]:

$$e \ co \ e$$
$$e \ co \ f \Leftrightarrow f \ co \ e$$
$$e \ co \ f \ \& \ f \ co \ h \Rightarrow e \ co \ h$$

Set $C(e)=\{f \in E(G) \mid f \ co \ e\}$, denoting the set of all co-distant edges in G. If the relation "co" is transitive on $C(e)$ then $C(e)$ is called an orthogonal cut "oc" of the graph G. Then G is called a *co-graph* and $E(G)$ being the union of disjoint orthogonal cuts.Let $m(G,c)$ be the number of qoc strips of length c in the graph G. Four counting polynomials have been defined [3-25] on the ground of qoc strips:

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

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

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

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

The first derivative (computed at $x=1$) of these counting polynomials provide interesting topological indices:

$$\Omega'(G,1)=\sum_c m(G,c)\times c=|E(G)|$$

$$\Theta'(G,1)=\sum_c m(G,c)\times c^2$$

$$Sd'(G,1)=\sum_c m(G,c)\times(|E(G)|-c)$$

$$\Pi'(G,1)=\sum_c m(G,c)\times c(|E(G)|-c)$$

The aim of this report is to compute the Theta polynomial and Theta index of V-phenylenic planar, nanotube and nanotori. Herein, our notation is standard and taken from the standard book of graph theory [26].

Results and Discussion

The structures of V-Phenylenic Planar, Nanotube and V-Phenylenic Nanotorus consist of several $C_4C_6C_8$ net. A $C_4C_6C_8$ net is a trivalent decoration made by alternating C_4, C_6 and C_8. Phenylenes are polycyclic conjugated molecules, composed of four-and six-membered rings such that every four membered ring (= square) is adjacent to two six-membered rings (= hexagons) [27-32]. Following *M.V. Diudea* [33] we denote a V-Phenylenic nanotube and V-Phenylenic nanotorus by $G=VPHX[m,n]$ and $H=VPHY[m,n]$, respectively and also denote a V-Phenylenic planar by $K=VPHP[m,n]$. A general representation of thees molecular graph are shown in Figure 1, Figure 2 and Figure 3. In Refs [34-47] some topological indices of V-phenylenic nanotube and V-phenylenic nanotori are computed.

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Theorem 1. Consider the V-Phenylenic Planar *K=VPHP[m,n]* $(\forall m,n\in \mathbb{N})$, the Theta polynomial of *VPHP[m,n]* is calculated by formulas:

- $\forall\ m\geq n,\ \Theta(VPHP[m,n],x) = 2nmx^{2m}+2n\left(3m-2n+1\right)x^{2n}+8\sum_{i=1}^{n-1} ix^{2i}+m\left(n-1\right)x^{m}$
- $\forall\ m<n,\ \Theta(VPHP[m,n],x) = 2n\left(m-1\right)x^{2n}+2m\left(2n-2m+3\right)x^{2m}+8\sum_{i=1}^{m-1} ix^{2i}+m\left(n-1\right)x^{m}$

Then the Theta index of *VPHP[m,n]* is

- $\forall\ m\geq n,\ \Theta(VPHP[m,n]) = 5nm^2+12mn^2-\frac{8}{3}n^3-4n^2-m^2+\frac{8}{3}n$
- $\forall\ m<n,\ \Theta(VPHP[m,n]) = 9nm^2+4mn^2-\frac{8}{3}m^3+3m^2-4n^2+\frac{8}{3}n$

Proof of Theorem 1. Let *K=VPHP[m,n]* be the V-Phenylenic Planar, with *6mn* vertices and *9mn-2n-m* edges. To compute the Theta polynomial of *K*, it is enough to calculate *C(e)* for every *e* in *E(K)*. By using the result herein [7] and from Figures 1, one can see that there are four types of edges-cut of *K* We denote the corresponding edges-cut by C_i *(i=1,... Max{m,n})* and C_i *(i=1,2,3)*. By definition of Theya polynomial and Tables 1 and 2, we have

$$\forall\ m\geq n:\ \Theta(VPHP[m,n],x)=\sum_{c} \mathrm{m}\left(VPHP[m,n],c\right).c.x^{c}$$

$$=4\sum_{i=1}^{n-1}\left(2i\right)x^{2i}+4n(m-n+1)x^{2n}+2nmx^{2m}+2n\left(m-1\right)x^{2n}+m\left(n-1\right)x^{m}$$

$$=2nmx^{2m}+2n\left(3m-2n+1\right)x^{2n}+8\sum_{i=1}^{n-1} ix^{2i}+m\left(n-1\right)x^{m}$$

Table 1: The number of co-distant edges, when *m≥n.*

Type of edges-cut	Number of co-distant edges	No
C_1	*2m*	*n*
C_2	*m*	*n-1*
C_3	*2n*	*m-1*
C_i $\forall$ *i=1,…,n-1*	*2i*	*4*
C_h	*2n*	*4(m-n+1)*

$$\forall\ m<n:\ \Theta(VPHP[m,n],x) = 4\sum_{i=1}^{m-1}\left(2i\right)x^{2i}+4m(n-m+1)x^{2m}+2nmx^{2m}+2n\left(m-1\right)x^{2n}+m\left(n-1\right)x^{m}$$

$$=2n\left(m-1\right)x^{2n}+2m\left(2n-2m+3\right)x^{2m}+8\sum_{i=1}^{m-1} ix^{2i}+m\left(n-1\right)x^{m}$$

Also, $\forall\ m\geq n$:

$$\Theta'\left(VPHP[m,n],x\right)|_{x=1} = \frac{\partial\left(2nmx^{2m}+2n\left(3m-2n+1\right)x^{2n}+8\sum_{i=1}^{n-1} ix^{2i}+m\left(n-1\right)x^{m}\right)}{\partial x}|_{x=1}$$

$$=4nm^2+4n^2\left(3m-2n+1\right)+16\sum_{i=1}^{n-1} i^2+\left(n-1\right)m^2$$

$$=5nm^2+12mn^2-8n^3+4n^2-m^2+16\underbrace{\sum_{i=1}^{n-1} i^2}_{8/3(2n^3-3n^2+n)}$$

$$=5nm^2+12mn^2-\tfrac{8}{3}n^3-4n^2-m^2+\tfrac{8}{3}n$$

Table 2: The number of co-distant edges, when $m<n$.

Type of edges-cut	Number of co-distant edges	No
C_1	$2m$	n
C_2	m	$n-1$
C_3	$2n$	$m-1$
C_i $\forall\ i=1,\ldots,m-1$	$2i$	4
C_m	$2m$	$4(n-m+1)$

And also $\forall\ m<n$:

$$\Theta(VPHP[m,n])=\frac{\partial\left(2n(m-1)x^{2n}+2m(2n-2m+3)x^{2m}+8\sum_{i=1}^{m-1}ix^{2i}+m(n-1)x^{m}\right)}{\partial x}\Bigg|_{x=1}$$

$$=9nm^2+4mn^2-\tfrac{8}{3}m^3+3m^2-4n^2+\tfrac{8}{3}n$$

Here the proof is completed. □

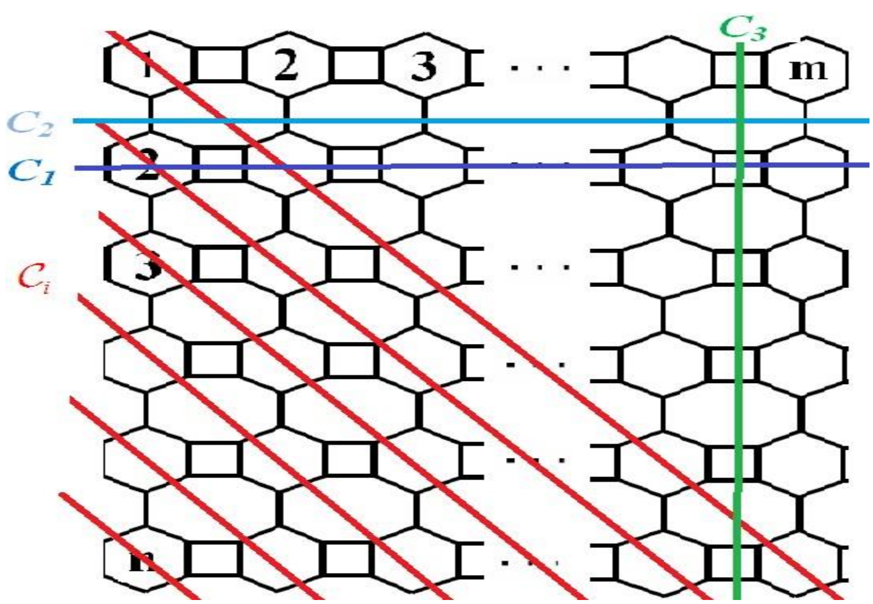

Figure 1: The 2-Dimetional Graph V-Phenylenic Nanotube K=*VPHP[m,n]*.

Theorem 2. Let *G* be the V-Phenylenic nanotube *VPHX[m,n]* $(\forall m,n\in \mathbb{N})$, Then the Theta polynomial of *VPHX[m,n]* is equal to:

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

And also the Theta index of *VPHX[m,n]* is equal to:

$$\Theta(VPHX[m,n])=5nm^{2}+12mn^{2}+m^{2}$$

Proof of Theorem 2. Let *G=VPHX[m,n]* be the V-Phenylenic nanotube, with *6mn* vertices and *9mn-m* edges. From Figures 2 and by using the results in reference [7], it is east to see that there are four types of edges-cut in *G*. We denote the corresponding edges-cut by C_i *(i=1,2,3)* and C. By definition of Theya polynomial and Tables 3, one can see that

$$\Theta(VPHX[m,n],x)=\sum_{c}\mathrm{m}\left(VPHX\left[m,n\right],c\right).c.\mathrm{x}^{c}$$
$$=2mnx^{2m}+m(n-1)x^{m}+2mnx^{2n}+4mnx^{2n}$$
$$=2mnx^{2m}+6mnx^{2n}+m(n-1)x^{m}$$

By definition of Theya index, we have

$$\Theta(VPHX[m,n])=\frac{\partial\left(2mnx^{2m}+6nmx^{2n}+m\left(n-1\right)x^{m}\right)}{\partial x}\Big|_{x=1}=5nm^{2}+12mn^{2}+m^{2}$$

Table 3: The number of co-distant edges, when *m≥n.*

Type of edges-cut	Number of co-distant edges	No
C_1	*2m*	*n*
C_2	*m*	*n-1*
C_3	*2n*	*m*
C	*2n*	*2m*

and this completes the proof.■

Theorem 3. Consider the V-Phenylenic Nanotori *H=VPHY[m,n]* with *6mn* vertices/atoms and *9mn* edges/bonds for all integer number *m,n.* Theta polynomial and Theta index of *H* are equal to:

$$\Theta(VPHY[m,n],x)=2nmx^{2m}+2n\left(3m-2n+1\right)x^{2n}+8\sum_{i=1}^{n-1}i\mathrm{x}^{2i}+m\left(n-1\right)x^{m}$$

$$\Theta(VPHY[m,n])=9nm^{2}+4mn^{2}-{}^{8}\!/_{3}\,m^{3+}3m^{2}-4n^{2+}\,{}^{8}\!/_{3}\,n$$

Proof. From Figure 3 and Table 4, the proof is analogous to the above proofs.

$$\Theta(VPHY[m,n],x)=\sum_{c}m\left(VPHY\left[m,n\right],c\right).c.\mathrm{x}^{c}$$
$$=4mnx^{2nm}+2mnx^{2m}+2mnx^{2n}+m(n-1)x^{m}$$

And $\Theta(VPHY[m,n])=8m^{2}n^{2}+5nm^{2}+4mn^{2}-m^{2}$. ■

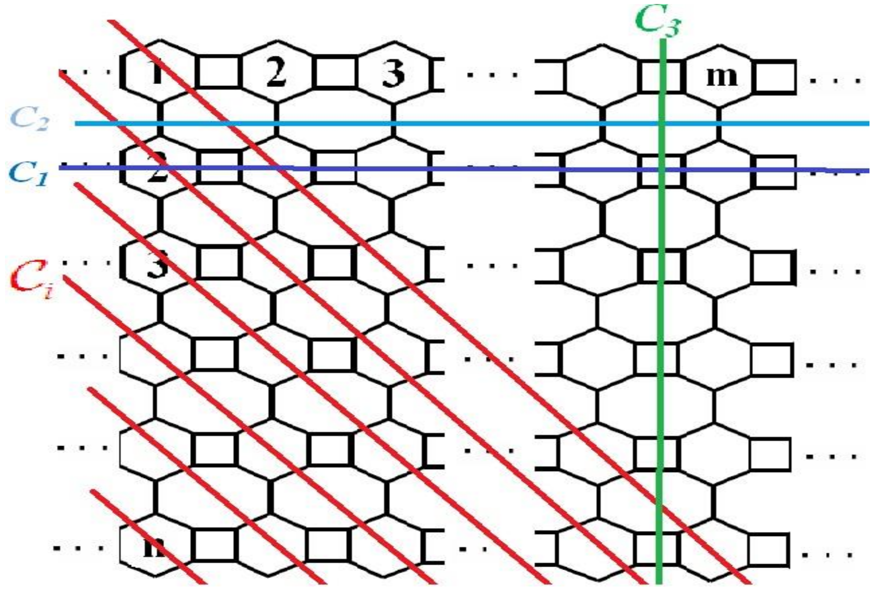

Figure 2: The 2-Dimetional Graph V-Phenylenic Nanotube G=*VPHX[m,n]*.

Table 4: The number of co-distant edges, when $m \geq n$.

Type of edges-cut	Number of co-distant edges	No
C_1	$2m$	n
C_2	m	$n-1$
C_3	$2n$	m
C	$2nm$	2

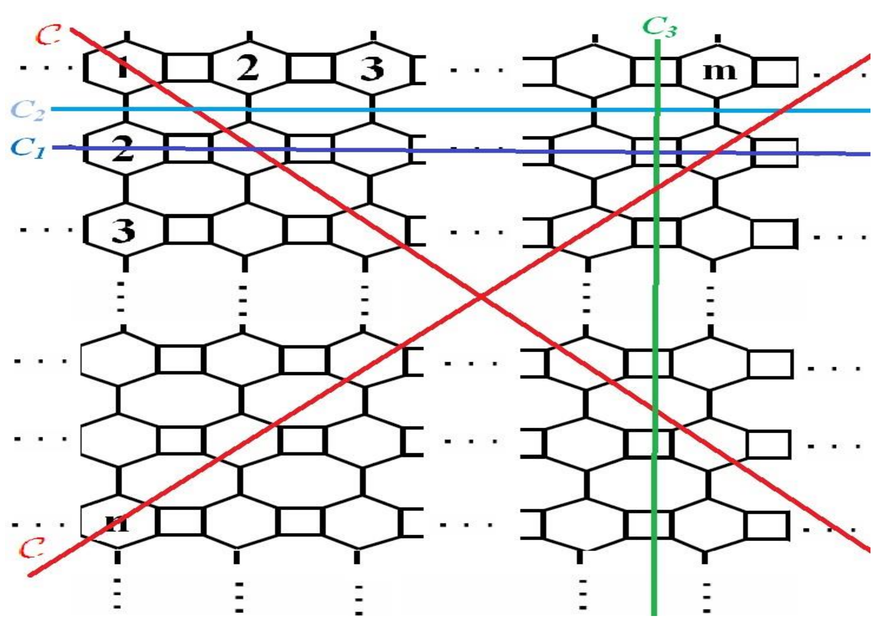

Figure 3: The 2-Dimetional Graph V-Phenylenic Nanotube H=*VPHY[m,n]*.

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