Computing omega and Sadhana polynomials of carbon nanotubes

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Counting polynomials are those polynomials having at exponent the extent of a property partition and coefficients the multiplicity/occurrence of the corresponding partition. In this paper, omega and Sadhana polynomials are computed for nanotubes. These polynomials were proposed on the ground of quasi-orthogonal cuts edge strips in polycyclic graphs. These counting polynomials are useful in the topological description of bipartite structures as well as in counting some single number descriptors, i.e. topological indices. These polynomials count equidistant and non-equidistant edges in graphs. In this paper, analytical closed formulas of these polynomials for H-Naphtalenic, $TUC_4C_8(R)[m,n]$ and $TUC_4[m,n]$ nanotubes are derived.

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1. Introduction and preliminary results

Mathematical chemistry is a branch of theoretical chemistry in which we discuss and predict the chemical structure by using mathematical tools and doesn't necessarily refer to the quantum mechanics. *Chemical graph theory* is a branch of mathematical chemistry in which we apply tools from graph theory to model the chemical phenomenon mathematically. This theory contributes a prominent role in the fields of chemical sciences.

Carbon nanotubes (CNTs) are types of nanostructure which are allotropes of carbon and having a cylindrical shape. Carbon nanotubes, a type of fullerene, have potential in fields such as nanotechnology, electronics, optics, materials science, and architecture. Carbon nanotubes provide a certain potential for metal-free catalysis of inorganic and organic reactions.

Counting polynomials are those polynomials having at exponent the extent of a property partition and coefficients the multiplicity/occurrence of the corresponding partition. A counting polynomial is defined as:

$$P(G,x) = \sum_k m(G,k)x^k \qquad (1)$$

Where the coefficient $m(G,k)$ are calculable by various methods, techniques and algorithms. The expression (1) was found independently by Sachs, Harary, Mili c′ , Spialter, Hosoya, etc [5]. The corresponding topological index $P(G)$ is defined in this way:

$$P(G) = P'(G,x)|_{x=1} = \sum_k m(G,k)\times k$$

A *moleculer/chemical graph* is a simple finite graph in which vertices denote the atoms and edges denote the chemical bonds in underlying chemical structure. This is more important to say that the hydrogen atoms are often omitted in any molecular graph. A graph can be represented by a matrix, a sequence, a polynomial and a numeric number (often called a topological index) which represents the whole graph and these representations are aimed to be uniquely defined for that graph.

Two edges $e = uv$ and $f = xy$ in $E(G)$ are said to be *codistant*, usually denoted by $e \; co \; f$, if

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

and

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

The relation "co" is reflexive as $e \; co \; e$ is true for all edges in G, also symmetric as if $e \; co \; f$ then $f \; co \; e$ for all $e, f \in E(G)$ but the relation "co" is not necessarily transitive. Consider

$$C(e) = \{ f \in E(G) : f \; co \; e\}$$

If the relation is transitive on $C(e)$ also, then $C(e)$ is called an *orthogonal cut* "co" of the graph G. Let $e = uv$ and $f = xy$ be two edges of a graph G, which are opposite or topological parallel, and this relation is denoted by $e \; op \; f$. A set of opposite edges, within the same face or ring, eventually forming a strip of adjacent faces/rings, is called an opposite edge strip ops, which is a quasi-orthogonal cut qoc (i.e. the transitivity relation is not necessarily obeyed). Note that "co" relation is defined in the whole graph while "op" is defined only in a face/ring.

In this article, G is considered to be simple connected graph with vertex set $V(G)$ and edge set $E(G)$, while $m(G,k)$ be the number of ops of length k, and $e = |E(G)|$ is the edge cardinality of G.

The omega polynomial was introduced by *Diudea* et al. in 2006 on the ground of op strips. The omega polynomial is proposed to describe cycle-containing molecular structures, particularly those associated with nanostructures.

Definition 1.1. [1] Let G be a graph, then its omega polynomial denoted by $\Omega(G,x)$ in x is defined as

$$\Omega(G,x) = \sum_k m(G,k) \times x^k$$

The Sadhana polynomial is defined based on counting opposite edge strips in any graph. This polynomial counts equidistant edges in G.

Definition 1.2. [6] Let G be a graph, then Sadhana polynomial denoted by $Sd(G,x)$ is defined as

$$Sd(G,x) = \sum_k m(G,k) \times x^{e-k}$$

Ashrafi et al. computed Sadhana polynomial of V-phenylenic nanotube and nanotori.

Theorem 1.0.1. [2] Let G be the graph of V-phenylenic nanotube, then Sadhana polynomial of G is

$$Sd(G,x) = 4 \sum_{i=1}^{Max\{m,n\}-1} x^{|E(G)|-2i} + 2(|n-m|+1)x^{|E(G)|-2Min\{m,n\}} +$$

$$nx^{|E(G)|-2m} + (m-1)x^{|E(G)|-2m} + (n-1)x^{|E(G)|-n}$$

All nanotubes are allotropes of carbon and are a type of fullerene. Ghorbani et al. computed omega and Sadhana polynomials of an infinite family of fullerene C_{10n}, $n \geq 10$.

Theorem 1.0.2. [8] Consider the fullerene graph C_{10n}, $n \geq 10$. Then the omega and Sadhana polynomials of C_{10n} are computed as follows:

$$\Omega(C_{10n},x) = \begin{cases} 10x^3 + 10x^{\frac{n}{2}} + 10x^{n-3} 0.35cm, & 2 \mid n \\ 10x^3 + 5x^{\frac{n-3}{2}} + 5x^{\frac{n+3}{2}} + 10x^{n-3}, & 2 \text{ does not divide } n \end{cases}$$

$$Sd(C_{10n},x) = \begin{cases} 10x^{15n-3} + 10x^{\frac{29n}{2}} + 10x^{14n+3} 0.35cm, & 2 \mid n \\ 10x^{15n-3} + 5x^{\frac{29n+3}{2}} + 5x^{\frac{29n-3}{2}} + 10x^{14n+3}, & 2 \text{ does not divide } n \end{cases}$$

The preceding results are used to compute their corresponding topological indices which provides a good model correlating the certain physico-chemical properties of these carbon allotropes.

2. Results and discussion

In this paper, we compute Omega and Sadhana polynomials of H-Naphtalenic, $TUC_4C_8(R)[m,n]$ and $TUC_4[p,q]$ nanotubes. For further study of these polynomials, their topological indices and various nanotubes, consult [3, 7, 9, 10, 11, 12, 13]. These polynomials are used to predict various physico-chemical properties of certain chemical compounds.

2.1 Results for H-Naphtalenic nanotubes

In this section, we compute omega and Sadhana polynomials forH-Naphtalenic nanotubes. This nanotube is a trivalent decoration having plane tiling of C_4, C_6 and C_8. This type of tiling can either cover a cylinder or a torus. This family of nanotubes is usually symbolized as $NPHX[m,n]$, in which m is the number of pairs of hexagons in first row and n is the number of alternative hexagons in a column. We have $|V(NPHX[m,n])| = 10mn$ and $|E(NPHX[m,n])| = 15mn - 2m$.

Now we compute omega polynomial of H-Naphtalenic nanotube.

Theorem 2.1.1. The Omega polynomial of H-Naphtalenic nanotube $NPHX[m,n]$, $\forall \; m,n \in \mathbb{N}$ is equal to:

$$\Omega(NPHX[m,n],x) = \begin{cases} \eta + 4\sum_{i=1}^{\lfloor \frac{n}{2} \rfloor -1} x^{2i} + 2(n-2m+1)x^{4m}, & m \leq \lfloor \frac{n}{2} \rfloor \\ \eta + 4\sum_{i=1}^{n-1} x^{2i} + 2(2m-n+1)x^{2n}, & m > \lfloor \frac{n}{2} \rfloor \end{cases}$$

where $\eta = nx^{3m} + mx^{2n} + (n-1)x^{2m}$.

Proof. Let G be the graph of H-Naphtalenic nanotube $NPHX[m,n]$, $\forall\ m,n \in \mathbb{N}$ with vertex set and edge set cardinalities are $10mn$ and $15mn-2m$ respectively. Table 1 shows the number of co-distant edges in G for $m \le \lfloor \frac{n}{2} \rfloor$, Table 2 shows the number of co-distant edges in G for $m > \lfloor \frac{n}{2} \rfloor$. The horizontal and vertical quasi-orthogonal cuts (qoc) are depicted in Fig.$1a$, while oblique qoc's are depicted in Fig $1b$. The oblique qoc's for e_4 and e_5 are same.

By using Table 1 and 2, the proof is straightforward.

Table 1. Number of co-distant edges of H-Naphtalenic nanotube $NPHX[m,n]$ *when* $m \le \lfloor \frac{n}{2} \rfloor$.

Types of qoc	Types of edges	No of co-distant edges	No of qoc
C_1	e_1	$3m$	n
C_2	e_2	$2n$	m
C_3	e_3	$2m$	$n-1$
C_k, where $k = 1,2,\ldots,\ j$	e_k where $k = 4,5$	$2i$ where $i = 1,2,\ldots,\lfloor \frac{n}{2} \rfloor - 1$	2
		$4m$	$n-2m+1$

Table 2. Number of co-distant edges of H-Naphtalenic nanotube $NPHX[m,n]$ *when* $m > \lfloor \frac{n}{2} \rfloor$.

Types of qoc	Types of edges	No of co-distant edges	No of qoc
C_1	e_1	$3m$	n
C_2	e_2	$2n$	m
C_3	e_3	$2m$	$n-1$
C_k, where $k = 1,2,\ldots, j$	e_k where $k = 4,5$	$2i$ where $i = 1,2,\ldots,n-1$	2
		$2n$	$2m-n+1$

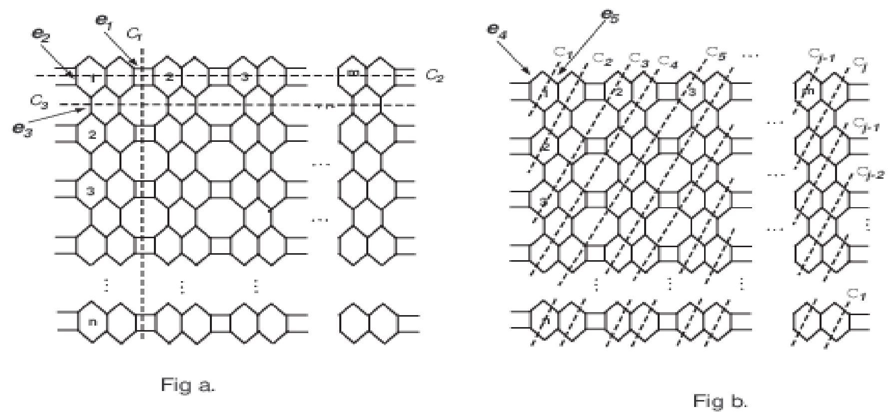

Fig. 1. Fig 1a. The horizontal and vertical qoc's, where Fig 1b. The oblique qoc's.

Now we apply formula and do some easy calculation to get our result.

$$\Omega(G,x)=\sum_k m(G,k)\times x^k$$

For $m \le \lfloor \frac{n}{2} \rfloor$

$$\Omega(G,x)=nx^{3m}+mx^{2n}+(n-1)x^{2m}+$$
$$2\{2\sum_{i=1}^{\lfloor \frac{n}{2}\rfloor -1} x^{2i}+(n-2m+1)x^{4m}\}$$

$$\Rightarrow \Omega(G,x)=nx^{3m}+mx^{2n}+(n-1)x^{2m}+2(n-2m+1)x^{4m}+$$
$$4x^2+4x^4+...+4x^{2\lfloor \frac{n}{2}\rfloor -2}$$

For $m > \lfloor \frac{n}{2} \rfloor$

$$\Omega(G,x)=nx^{3m}+mx^{2n}+(n-1)x^{2m}+$$
$$2\{2\sum_{i=1}^{n-1} x^{2i}+(2m-n+1)x^{2n}\}$$

$$\Rightarrow \Omega(G,x)=nx^{3m}+mx^{2n}+(n-1)x^{2m}+2(2m-n+1)x^{2n}+$$
$$4x^2+4x^4+...+4x^{2n-2}.$$

In the following theorem, the Sadhana polynomial of H-Naphtalenic nanotube $NPHX[m,n]$ is computed.

Theorem 2.1.2. The Sadhana polynomial of H-Naphtalenic nanotube

$NPHX[m,n]$, $\forall\ m,n \in \mathrm{N}$ is as follows:

$$Sd(NPHX[m,n],x)=\begin{cases}\eta+4\sum_{i=1}^{\lfloor \frac{n}{2}\rfloor -1} x^{15mn-2m-2i}+ & \\ 2(n-2m+1)x^{15mn-6m}, & m\le\lfloor \frac{n}{2}\rfloor \\ \eta+4\sum_{i=1}^{n-1} x^{15mn-2m-2i}+ & \\ 2(2m-n+1)x^{15mn-2m-2n}, & m>\lfloor \frac{n}{2}\rfloor\end{cases}$$

where

$$\eta=nx^{15mn-5m}+mx^{15mn-2m-2n}+(n-1)x^{15mn-4m}.$$

Proof. Let G be the graph of H-Naphtalenic nanotube $NPHX[m,n]$, $\forall\ m,n\in \mathrm{N}$ with vertex set and edge set cardinalities are $10mn$ and $15mn-2m$ respectively.

By using Table 1 and 2 the proof is easy. Now we apply formula and do some computation to get our result.

$$Sd(G,x)=\sum_k m(G,k)\times x^{e-k}$$

For $m \le \lfloor \frac{n}{2} \rfloor$

$$Sd(G,x)=nx^{15mn-5m}+mx^{15mn-2m-2n}+(n-1)x^{15mn-4m}+$$
$$2\{2\sum_{i=1}^{\lfloor \frac{n}{2}\rfloor -1} x^{15mn-2m-2i}+(n-2m+1)x^{15mn-6m}\}$$

$$\Rightarrow Sd(G,x)=nx^{15mn-5m}+mx^{15mn-2m-2n}+(n-1)x^{15mn-4m}+$$
$$2(n-2m+1)x^{15mn-6m}+4x^{15mn-2m-2}+$$
$$4x^{15mn-2m-4}+...+4x^{15mn-2m-2\lfloor \frac{n}{2}\rfloor -2}$$

For $m > \lfloor \frac{n}{2} \rfloor$

$$Sd(G,x)=nx^{15mn-5m}+mx^{15mn-2m-2n}+(n-1)x^{15mn-4m}+$$
$$2\{2\sum_{i=1}^{n-1} x^{15mn-2m-2i}+(2m-n+1)x^{15mn-2m-2n}\}$$

$$\Rightarrow Sd(G,x)=nx^{15mn-5m}+mx^{15mn-2m-2n}+(n-1)x^{15mn-4m}+$$
$$2(2m-n+1)x^{15mn-2m-2n}+4x^{15mn-2m-2}+$$
$$4x^{15mn-2m-4}+...+4x^{15mn-2m-2n+2}$$

2.2 Results for $TUC_4C_8(R)[m,n]$, $\forall\ m,n\in \mathrm{N}$ nanotube

In this section, we determine omega and Sadhana polynomials for $TUC_4C_8(R)[m,n]$, $\forall\ m,n\in \mathrm{N}$ nanotube. This nanotube is a trivalent decoration having plane tiling of C_4 and C_8. In other words, the whole lattice is a plane tiling of C_4 and C_8 and this type of tiling can either cover a cylinder or a torus. In $TUC_4C_8(R)[m,n]$ nanotube, m is the number of octagons in any row and n is the number of octagons in any column. We have $|V(TUC_4C_8(R)[m,n])| = 4m(n+1)$ and $|E(TUC_4C_8(R)[m,n])| = 6mn+5m$.

In the following theorem, the omega polynomial of $TUC_4C_8(R)[m,n]$ nanotube is computed.

Theorem 2.2.1. The omega polynomial of $TUC_4C_8(R)[m,n]$ nanotube $\forall\ m,n \in \mathbb{N}$, is as follows:

$$\Omega(TUC_4C_8(R)[m,n],x) = \begin{cases} \eta + 4\sum_{i=1}^{n} x^{2i} + 2(m-n+1)x^{2n+2}, & m \geq n \\ \eta + 4\sum_{i=1}^{m} x^{2i} + 2(n-m+1)x^{2m+2}, & m < n \end{cases}$$

where $\eta = mx^{n+1} + nx^{m+1}$.

Proof. Let G be the graph of $TUC_4C_8(R)[m,n]$ nanotube, $\forall\ m,n \in \mathbb{N}$. Table 3 shows the number of co-distant edges in G for $m \geq n$ and table 4 shows the number of co-distant edges in G for $m < n$. The quasi-orthogonal cuts are depicted in Fig 2. The oblique qoc's for e_3 and e_4 are same.

Table 3. Number of co-distant edges of $TUC_4C_8(R)[m,n]$ nanotube, when $m \geq n$.

Types of qoc's	Types of edges	No of co-distant edges	No of qoc
C_1	e_1	$n+1$	m
C_2	e_2	$m+1$	n
C_k where $k = 1,2,..., j$	e_k where $k = 3,4$	$2i$ where $i = 1,2,...,n$	2
		$2n+2$	$m-n+1$

Table 4. Number of co-distant edges of $TUC_4C_8(R)[m,n]$ nanotube, when $m < n$.

Types of qoc's	Types of edges	No of co-distant edges	No of qoc
C_1	e_1	$n+1$	m
C_2	e_2	$m+1$	n
C_k where $k = 1,2,..., j$	e_k where $k = 3,4$	$2i$ where $i = 1,2,...,m$	2
		$2m+2$	$n-m+1$

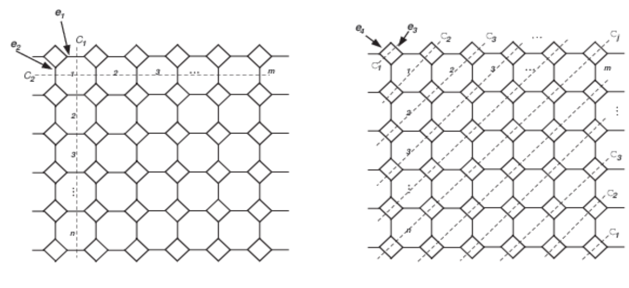

Fig 4a: Fig 4b:

Fig. 2. Fig 2a. The horizontal and vertical qoc's, where Fig 2b. The oblique qoc's.

By using Table 3 and 4 the proof is mechanical. Now we apply formula and do some calculation to get our result.

$$\Omega(G,x) = \sum_k m(G,k) \times x^k$$

For $m \geq n$

$$\Omega(G,x) = mx^{n+1} + nx^{m+1} + 2\{2\sum_{i=1}^{n} x^{2i} + (m-n+1)x^{2n+2}\}$$

$$\Rightarrow \Omega(G,x) = mx^{n+1} + nx^{m+1} + 2(m-n+1)x^{2n+2} + 4x^2 + 4x^4 + ... + 4x^{2n}$$

For $m < n$

$$\Omega(G,x) = mx^{n+1} + nx^{m+1} + 2\{2\sum_{i=1}^{m} x^{2i} + (n-m+1)x^{2m+2}\}$$

$$\Rightarrow \Omega(G,x) = mx^{n+1} + nx^{m+1} + 2(n-m+1)x^{2m+2} + 4x^2 + 4x^4 + ... + 4x^{2m}$$

Now we compute Sadhana polynomial of

$TUC_4C_8(R)[m,n]$, nanotube $\forall\ m,n\in\mathbb{N}$. Following theorem shows the Sadhana polynomial for this family of nanotubes.

Theorem 2.2.2. Consider the graph of $TUC_4C_8(R)[m,n]$, nanotube, $\forall\ m,n\in\mathbb{N}$. Then its Sadhana polynomial is as follows:

$$Sd(TUC_4C_8(R)[m,n],x)=\begin{cases}\eta+4\sum_{i=1}^{n}x^{6mn+5m-2i} \\ +2(m-n+1)x^{6mn+5m-2n-2}, & m\ge n \\ \eta+4\sum_{i=1}^{m}x^{6mn+5m-2i} \\ +2(n-m+1)x^{6mn+3m-2}, & m<n\end{cases}$$

where $\eta=mx^{6mn+5m-n-1}+nx^{6mn+4m-1}$.

Proof. Let G be the graph of $TUC_4C_8(R)[m,n]$, nanotube $\forall\ m,n\in\mathbb{N}$. The proof of this result is just calculation based. We prove it by using Table 3 and 4. We know that

$$Sd(G,x)=\sum_k m(G,k)\times x^{e-k}$$

For $m\ge n$

$$Sd(G,x)=mx^{6mn+5m-n-1}+nx^{6mn+4m-1}+$$

$$2\{2\sum_{i=1}^{n}x^{6mn+5m-2i}+(m-n+1)x^{6mn+5m-2n-2}\}$$

$$\Rightarrow Sd(G,x)=mx^{6mn+5m-n-1}+nx^{6mn+4m-1}+2(m-n+1)x^{6mn+5m-2n-2}+$$

$$4x^{6mn+5m-2}+4x^{6mn+5m-4}+...+4x^{6mn+5m-2n}$$

For $m<n$

$$Sd(G,x)=mx^{6mn+5m-n-1}+nx^{6mn+4m-1}+$$

$$2\{2\sum_{i=1}^{m}x^{6mn+5m-2i}+(n-m+1)x^{6mn+3m-2}\}$$

$$\Rightarrow Sd(G,x)=mx^{6mn+5m-n-1}+nx^{6mn+4m-1}+2(n-m+1)x^{6mn+3m-2}+$$

$$4x^{6mn+5m-2}+8x^{6mn+5m-4}+...+4x^{6mn+3m}$$

2.3 Results for $TUC_4[m,n]$, $\forall\ m,n\in\mathbb{N}$ nanotube

In this section, we compute omega and Sadhana polynomials of nanotube covered only by C_4. The $2D$-lattice of this nanotube is a plane tiling of C_4. This tessellation of C_4 can either cover a cylinder or a torus. This nanotube is denoted by $TUC_4[m,n]$, in which m is the number of squares in any row and n is the number of squares in any column as shown in Fig. 4. A $3D$ representation of $TUC_4[6,n]$ nanotube is depicted in Fig. 3.

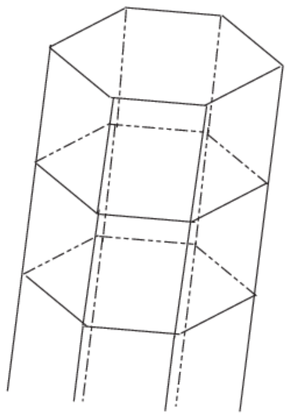

Fig. 3. A $TUC_4[6,n]$ nanotube covered by C_4.

Lemma 2.3.1. Let $TUC_4[m,n]$ be the graph of nanotube covered by C_4, then its number of vertices are

$$|V(TUC_4[m,n])|=(n+1)(m+1)$$

Lemma 2.3.2. Consider the graph of $TUC_4[m,n]$ nanotube with, then its edge set cardinality is

$$|E(NPHX[m,n])|=(2n+1)(m+1)$$

Now we compute omega polynomial of $TUC_4[m,n]$ nanotube.

Theorem 2.3.1. The omega polynomial of $TUC_4[m,n]$, $\forall\ m,n\in\mathbb{N}$ is equal to

$$\Omega(TUC_4[m,n],x)=\begin{cases}nx^{m+1}+(m+1)x^{n+1}, & m\ne n \\ (2m+1)x^{m+1}, & m=n\end{cases}$$

Proof. Let G be the graph of $TUC_4[m,n]$, $\forall\ m,n\in\mathbb{N}$ nanotube with vertex and edge cardinalities are $(n+1)(m+1)$ and $(2n+1)(m+1)$ respectively. Table 5 shows the number of co-distant edges of G with $m\ne n$ and Fig. 4 shows the quasi-orthogonal cuts of G with $m\ne n$.

Table 5. Quasi-orthogonal cuts of $TUC_4[m,n]$, $\forall\ m,n \in \mathbb{N}$ *nanotube with* $m \neq n$.

Types of qoc's	Types of edges	Number of co-distant edges	No of qoc
C_1	e_1	$m+1$	n
C_2	e_2	$n+1$	$m+1$

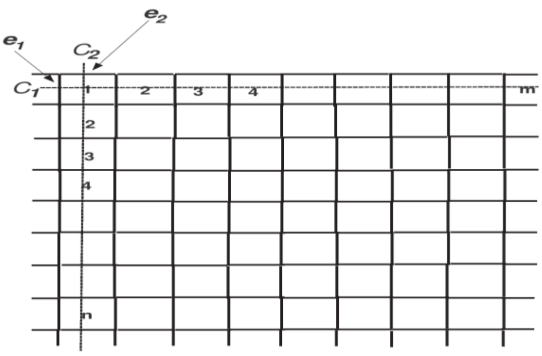

Fig. 4. Quasi-orthogonal cuts of $TUC_4[m,n]$, $\forall\ m,n \in \mathbb{N}$ *nanotubes with* $m \neq n$.

By using Table 5, the proof is just calculation based. Now we apply formula to get our required result.

$$\Omega(G,x) = \sum_k m(G,k) \times x^k$$

For $m \neq n$,

$$\Omega(G,x) = nx^{m+1} + (m+1)x^{n+1}$$

By just putting $m = n$ in preceding equation, we get our second part of result.

Now we compute Sadhana polynomial of $TUC_4[m,n]$, $\forall\ m,n \in \mathbb{N}$.

Theorem 2.3.2. The Sadhana polynomial of $TUC_4[m,n]$, $\forall\ m,n \in \mathbb{N}$ is equal to

$$Sd(TUC_4[m,n],x) = \begin{cases} nx^{2mn+2n} + (m+1)x^{2mn+m+n}, & m \neq n \\ (2m+1)x^{2m^2+2m}, & m = n \end{cases}$$

Proof. Let G be the graph of $TUC_4[m,n]$, $\forall$ $m,n \in \mathbb{N}$ nanotube with vertex and edge cardinalities are $(n+1)(m+1)$ and $(2n+1)(m+1)$ respectively.

By using Table 5, the proof is quite easy. We know that

$$Sd(G,x) = \sum_k m(G,k) \times x^{e-k}$$

For $m \neq n$,

$$Sd(G,x) = nx^{2mn+2n} + (m+1)x^{2mn+m+n}$$

By just putting $m = n$ in preceding equation, we get our second part of result.

3. Conclusion and general remarks

In this paper, two important counting polynomials called omega and Sadhana are studied. These polynomials are useful in determining Omega and Sadhana topological indices which play an important role in QSAR/QSPR study. We computed these polynomials for H-Naphtalenicnanotube $NPHX[m,n]$, $TUC_4C_8(R)[m,n]$ nanotube and $TUC_4[m,n]$ nanotube, $\forall\ m,n \in \mathbb{N}$ for the first time.

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