Computing topological polynomials of certain nanostructures

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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, Sadhana and PI polynomials are computed for Multilayer Hex-Cells nanotubes, One Pentagonal Carbon nanocones and Melem Chain 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 Multi-layer Hex-Cells MLH (k, d) nanotubes, One Pentagonal Carbon CNC_5 (n) nanocones and Melem Chain MC (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:

$$P(G,x)=\sum_k m(G,k)x^k \tag{1}$$

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 $E(G)$, $m(G,k)$ be the number of ops of length k, $e = |E(G)|$ 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. *[6]* 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. *[8]* Let G be a graph, then Sadhana polynomial denoted by $Sd(G,x)$ is defined as

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

The PI polynomial is also defined based on counting opposite edge strips in any graph. This polynomial counts non-equidistant edges in G.

Definition 1.3. *[8]* Let G be a graph, then PI polynomial denoted by $PI(G,x)$ is defined as

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

Yazdani et al. determined Padmakar-Ivan (PI) polynomials of $HAC_5C_6C_7[4p,2q]$ nanotubes.

Theorem 1.0.1. *[21]* Let G be the $HAC_5C_6C_7$ nanotube, then PI polynomial of G is

$$PI(G,x) = qx^{9pq-\frac{p}{4}} + px^{9pq+\frac{p}{4}6q} + 4qx^{9pq-\frac{15}{4}p+2} - 9pq - \frac{p}{4} + \binom{|V(G)|+1}{2}$$

where $|V(G)| = \frac{3}{2}p^2q + \frac{7}{2}q + p$

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

Theorem 1.0.2. *[1]* 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 1.0.3. *[11]* Consider the fullerene graph C_{10n}, $n \geq 10$. Then the Omega and Sadhana polynomials of C_{10n} are computed as follows:

$$\Omega(C_{10n},x) = \begin{cases} 10x^3 + 10x^{\frac{n}{2}} + 10x^{n-3} 0.35cm & 2 \mid n \\ 10x^3 + 5x^{\frac{n-3}{2}} + 5x^{\frac{n+3}{2}} + 10x^{n-3} & 2 \nmid n \end{cases}$$

$$Sd(C_{10n},x) =$$

$$\begin{cases} 10x^{15n-3} + 10x^{\frac{29n}{2}} + 10x^{14n+3} 0.35cm & 2 \mid n \\ 10x^{15n-3} + 5x^{\frac{29n+3}{2}} + 5x^{\frac{29n-3}{2}} + 10x^{14n+3}, & 2 \nmid n \end{cases}$$

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, Sadhana and PI polynomials for Multilayer Hex-Cells MLH (k, d) nanotubes, One Pentagonal Carbon CNC_5 (n) nanocones and Melem Chain MC (n) nanotubes. For further study of these polynomials their topological indices and polynomials of various nanotubes, consult [3, 4, 7, 10, 12-18, 20]. These polynomials are used to predict various physico-chemical properties of certain chemical compounds.

2.1. Multilayer Hex-Cells MLH (k, d) nanotubes

In this section, we compute Omega, Sadhana and PI polynomials for MLH (k, d) nanotubes. A Hex-Cell nanotube [19] with depth d is denoted by HC (d) and can be constructed by using units of hexagon cells, each of six vertices. A Hex-Cell nanotube with depth d has d levels numbered from 1 to d, where level 1 represents the innermost level corresponding to one hexagon cell. Level 2 corresponds to the six hexagon cells surrounding the hexagon at level 1. Level 3 corresponds to the 12 hexagon cells surrounding the six hexagons at level 2 as shown in Figure 1. Each level i has V_i vertices, where $V_i = 6(2i - 1)$ and the total number of vertices in a Hex-Cell nanotubes HC (d) is $V = 6d^2$. The Multilayer Hex-Cell (MLH) is a modular interconnection network that consists of layers of identical Hex-Cells nanotubes connected together in hierarchical fashion as shown in Figure 2. The MLH is denoted by MLH (k, d), where k denotes the layer number, and d denotes the depth of the identical Hex-Cell. This family of nanotubes is usually symbolized as MLH (k, d). We have $|V(MLH(k, d))| = 6kd^2$ and $|E(MLH(k, d))| = 6(2k + \sum_{r=1}^{k-1} 2(k + r)) + 6kd^2$.

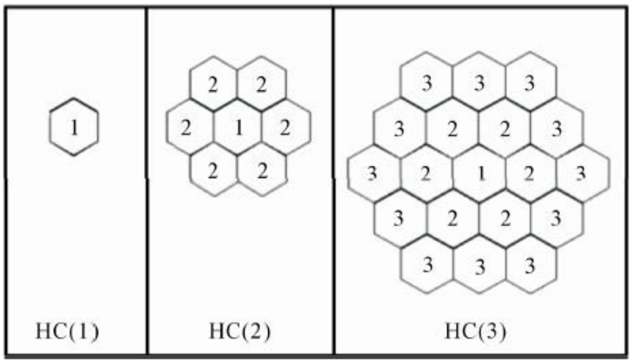

Fig. 1. (a) HC (one level) (b) (two levels) (c) (three levels).

Theorem 2.1.1. The Omega polynomial of MLH (k, d) nanotubes $\forall\ k, d \in \mathbb{N}$, is as follows:

$$\Omega\, MLH(k,d) = 6((2k-1) + 2\sum_{r=1}^{k-1}(2k-r-1)x^{2(2k+\sum_{r=1}^{k-1}2(k+r))} + (k-1)x^{6kd^2}).$$

Proof: Let G be the graph of MLH (k, d) nanotubes $\forall\ k, d \in \mathbb{N}$. Table 1 shows the number of co-distant edges in G. By using table 1 the proof is mechanical.

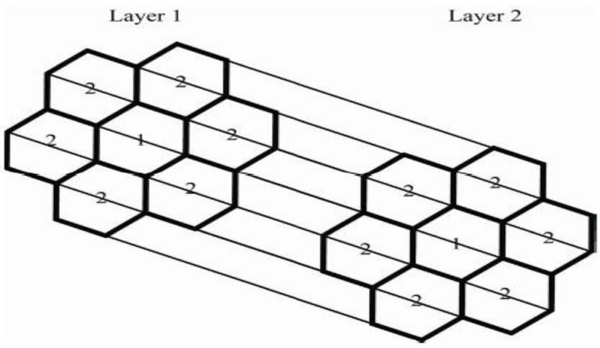

Fig. 2. MLH (2, 2).

Table 1. Number of co-distant edges of MLH (k,d) nanotube.

Types of qoc's	Types of edges	No of co-distant edges	No of qoc
C_1	e_1	$2k+\sum_{r=1}^{k-1}2(k+r)$	$2k-1+2\sum_{r=1}^{k-1}(2k-r-1)$
C_2	e_2	$2k+\sum_{r=1}^{k-1}2(k+r)$	$2k-1+2\sum_{r=1}^{k-1}(2k-r-1)$
C_3	e_3	$2k+\sum_{r=1}^{k-1}2(k+r)$	$2k-1+2\sum_{r=1}^{k-1}(2k-r-1)$
C_4	e_4	$6kd^2$	k-1

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

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

$$\Omega(G,x) = 2(2k-1) + 2\sum_{r=1}^{k-1}(2k-r-1)x^{2(2k+\sum_{r=1}^{k-1}2(k+r))} + 2(2k-1) + 2\sum_{r=1}^{k-1}(2k-r-1)x^{2(2k+\sum_{r=1}^{k-1}2(k+r))} +$$

$$2(2k-1) + 2\sum_{r=1}^{k-1}(2k-r-1)x^{2(2k+\sum_{r=1}^{k-1}2(k+r))} + (k-1)x^{6kd^2}$$

$$\Rightarrow \Omega(G,x) = 6((2k-1) + 2\sum_{r=1}^{k-1}(2k-r-1)x^{2(2k+\sum_{r=1}^{k-1}2(k+r))} + (k-1)x^{6kd^2})$$

Now we compute Sadhana polynomial of $MLH(k,d)$ nanotube $\forall\ k, d \in \mathbb{N}$. Following theorem shows the Sadhana polynomial for this family of nanotubes.

Theorem 2.1.2. Consider the graph of $MLH(k,d)$ nanotube $\forall\ k,d \in \mathbb{N}$. Then its Sadhana polynomial is as follows:

$$Sd(MLH(k,d),x) = 6((2k-1)+2\sum_{r=1}^{k-1}(2k-r-1))x^{4(2k+\sum_{r=1}^{k-1}2(k+r)+k6d^2)} + (k-1)x^{6(2k+\sum_{r=1}^{k-1}2(k+r))}$$

Proof. Let G be the graph of $MLH(k,d)$ nanotube $\forall\ k,d \in \mathbb{N}$. The proof of this result is just calculation based. We prove it by using table 1. We know that

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

$$Sd(G,x) = 2((2k-1)+2\sum_{r=1}^{k-1}(2k-r-1))x^{6(2k+\sum_{r=1}^{k-1}2(k+r)+6kd^2)-2(2k+\sum_{r=1}^{k-1}2(k+r))} +$$
$$2((2k-1)+2\sum_{r=1}^{k-1}(2k-r-1))x^{6(2k+\sum_{r=1}^{k-1}2(k+r)+6kd^2)-2(2k+\sum_{r=1}^{k-1}2(k+r))} + 2((2k-1)+$$
$$2\sum_{r=1}^{k-1}(2k-r-1))x^{6(2k+\sum_{r=1}^{k-1}2(k+r)+6kd^2)-2(2k+\sum_{r=1}^{k-1}2(k+r))} + (k-1)x^{6(2k+\sum_{r=1}^{k-1}2(k+r))+6kd^2-6kd^2}$$

$$\Rightarrow Sd(G,x) = 6((2k-1)+2\sum_{r=1}^{k-1}(2k-r-1))x^{4(2k+\sum_{r=1}^{k-1}2(k+r)+k6d^2)} + (k-1)x^{6(2k+\sum_{r=1}^{k-1}2(k+r))}$$

Next we compute PI polynomial of $MLH(k,d)$ nanotube. Following theorem explains the PI polynomial of this family of nanotubes.

Theorem 2.1.3. Consider the graph of $MLH(k,d)$ nanotube $\forall\ k,d \in \mathbb{N}$. Then its PI polynomial is as follows:

$$PI(MLH(k,d),x) = 12(2k(2k-1)+(2k-1)\sum_{r=1}^{k-1}2(k+r)+4k\sum_{r=1}^{k-1}(2k-r-1)+$$
$$2\sum_{r=1}^{k-1}(2k-r-1)(\sum_{r=1}^{k-1}2(k+r)))x^{4(2k+\sum_{r=1}^{k-1}2(k+r))+6kd^2} + 2(k-1)(2k+\sum_{r=1}^{k-1}2(k+r))x^{6(2k+\sum_{r=1}^{k-1}2(k+r))}$$

Proof. Let G be the graph of $MLH(k,d)$ nanotube $\forall\ k,d \in \mathbb{N}$. We prove it by using table 1. We know that

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

$$PI(G,x) = 2((2k-1)+2\sum_{r=1}^{k-1}(2k-r-1))\times 2(2k+\sum_{r=1}^{k-1}2(k+r)x^{6(2k+\sum_{r=1}^{k-1}2(k+r))+6kd^2-2(2k+\sum_{r=1}^{k-1}2(k+r))} +$$
$$2((2k-1)+2\sum_{r=1}^{k-1}(2k-r-1))\times 2(2k+\sum_{r=1}^{k-1}2(k+r)x^{6(2k+\sum_{r=1}^{k-1}2(k+r))+6kd^2-2(2k+\sum_{r=1}^{k-1}2(k+r))} +$$

$$2((2k-1)+2\sum_{r=1}^{k-1}(2k-r-1))\times 2(2k+\sum_{r=1}^{k-1}2(k+r)x^{6(2k+\sum_{r=1}^{k-1}2(k+r))+6kd^2-2(2k+\sum_{r=1}^{k-1}2(k+r))}+$$

$$2(k-1)(2k+\sum_{r=1}^{k-1}2(k+r))x^{6(2k+\sum_{r=1}^{k-1}2(k+r))+6kd^2-6kd^2}$$

$$\Rightarrow PI(G,x)=12(2k(2k-1)+(2k-1)\sum_{r=1}^{k-1}2(k+r)+4k\sum_{r=1}^{k-1}(2k-r-1)+$$

$$2\sum_{r=1}^{k-1}(2k-r-1)(\sum_{r=1}^{k-1}2(k+r)))x^{4(2k+\sum_{r=1}^{k-1}2(k+r))+6kd^2}+2(k-1)(2k+\sum_{r=1}^{k-1}2(k+r))x^{6(2k+\sum_{r=1}^{k-1}2(k+r))}$$

2.2 One pentagonal carbon $CNC_5(n)$ for $n\geq 3$ nanocones

In this section, we determine Omega, Sadhana and PI polynomials for $CNC_5(n)$, $n\geq 3$ nanocones. One pentagonal carbon nanocones, Fig. 3, originally discovered by Ge and Sattler in 1994 [9]. These are constructed from a graphene sheet by removing a 60^o wedge and joining the edges produces a cone with a single pentagonal defect at the apex. In $CNC_5(n)$ nanocone, the number of vertices and edges are $5n^2$ and $\frac{5}{2}n(3n-1)$ respectively.

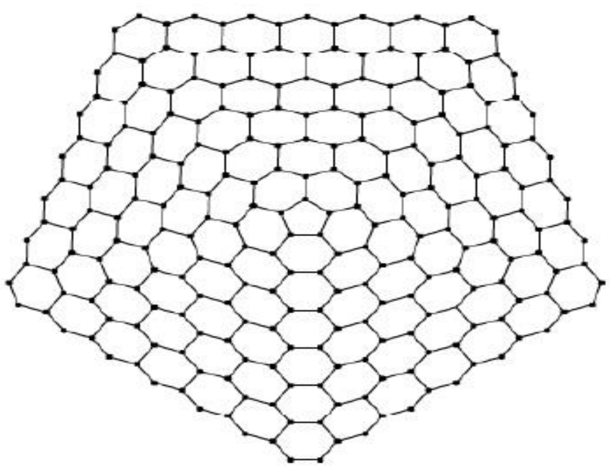

Fig. 3. A representation of $CNC_5(7)$ nanocone.

Now we compute Omega polynomial of $CNC_5(n)$ nanocone.

Theorem 2.2.1. The Omega polynomial of $CNC_5(n)$ nanocone for $n\geq 3$ is as follows:

$$\Omega(CNC_5(n),x)=5(x^{\sum_{i=1}^{n-2}(n+i)}+x^n(x^{n-1}+1))$$

Proof. Let G be the graph of one pentagonal carbon $CNC_5(n)$ for $n\geq 3$ nanocone. Table 2 shows the number of co-distant edges in G. By using table 2, the proof is straightforward.

Table 2. Number of co-distant edges of $CNC_5(n)$ for $n\geq 3$ nanocone.

Types of qoc	Types of edges	No. of co-distant edges	No. of qoc
C_1	e_1	n	5
C_2	e_2	$\sum_{i=1}^{n-2}(n+i)$	5
C_3	e_3	$2n-1$	5

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

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

$$\Omega(G,x)=5x^n+5x^{\sum_{i=1}^{n-2}(n+i)}+5x^{2n-1}$$

$$\Rightarrow \Omega(G,x)=5x^{\sum_{i=1}^{n-2}(n+i)}+5x^n(x^{n-1}+1)$$

$$\Rightarrow \Omega(G,x)=5(x^{\sum_{i=1}^{n-2}(n+i)}+x^n(x^{n-1}+1))$$

In the following theorem, the Sadhana polynomial of $CNC_5(n)$ for $n\geq 3$ nanocone is computed.

Theorem 2.2.2. The Sadhana polynomial of one pentagonal carbon $CNC_5(n)$ for $n\geq 3$ nanocone is as follows:

$$Sd(CNC_5(n),x)=5(x^{\frac{n}{2}(15n-7)}+x^{\frac{5}{2}n(3n-1)-\sum_{i=1}^{n-2}(n+i)}+x^{\frac{3}{2}(n(5n-3)+1)}$$

Proof. Let G be the graph of one pentagonal carbon $CNC_5(n)$ for $n\geq 3$ nanocone. By using table 2 the proof is easy. Now we apply formula and do some computation to get our result.

$$Sd(G,x)=5x^{\frac{5}{2}n(3n-1)-n}+5x^{\frac{5}{2}n(3n-1)-\sum_{i=1}^{n-2}(n+i)}+5x^{\frac{5}{2}n(3n-1)-(2n-1)}$$

$$\Rightarrow 5(x^{\frac{n}{2}(15n-7)}+x^{\frac{5}{2}n(3n-1)-\sum_{i=1}^{n-2}(n+i)}+x^{\frac{3}{2}(n(5n-3)+1)}$$

PI polynomial of one pentagonal carbon $CNC_5(n)$ for $n\geq 3$ nanocone is computed in [2].

2.3 Melem chain $MC(n)$ for $n\in\mathbb{N}$

In this section, we compute Omega, Sadhana and PI polynomials for melem $(2,5,8-triamino-tri-s-triazine)$ $C_6N_7(NH_2)_3$ chain nanotube. Melem was obtained as a crystalline powder by thermal treatment of different less condensed $C-N-H$ compounds (e.g., melamine $C_3N_3(NH_2)_3$, dicyandiamide $H_4C_2N_4$, ammonium dicyanamide $NH_4[N(CN)_2]$, or cyanamide H_2CN_2, respectively) at temperatures up to 450^oC in sealed glass ampules. The vertices and edges in Melem chain are $18n+4$ and $21n+3$ respectively. Now we compute Omega polynomial of melem chain $MC(n)$ nanotube.

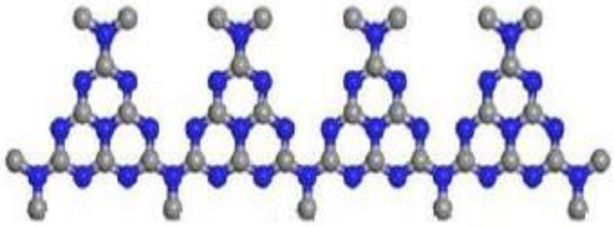

Fig. 4. A representation of $MC(4)$ nanotube.

Theorem 2.3.1. The Omega polynomial of nanotube $MC(n)$ for $n\in\mathbb{N}$ is equal to:

$$\Omega(MC(n),x)=(6n+5)x^{7n+1}$$

Proof. Let G be the graph of $MC(n)$ nanotube for $n\in\mathbb{N}$. Table 3 shows the number of co-distant edges in G. By using table 3 the proof is straightforward.

Table 3. Number of co-distant edges of $MC(n)$ nanotube.

Types of qoc	Types of edges	No. of co-distant edges	No. of qoc
C_1	e_1	$7n+1$	$3n+1$
C_2	e_2	$7n+1$	$3n+1$
C_3	e_3	$7n+1$	3

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

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

$$\Omega(G,x)=(3n+1)x^{7n+1}+(3n+1)x^{7n+1}+3x^{7n+1}$$

$$\Rightarrow \Omega(G,x)=(3n+1+3n+1+3)x^{7n+1}$$

$$\Rightarrow \Omega(G,x)=(6n+5)x^{7n+1}$$

In the following theorem, the Sadhana polynomial of $MC(n)$ nanotube is computed.

Theorem 2.3.2. The Sadhana polynomial of $MC(n)$ nanotube for $n\in\mathbb{N}$ is as follows:

$$Sd(,x)=(6n+5)^{2(7n+1)}$$

Proof. Let G be the graph $MC(n)$ nanotube for $n\in\mathbb{N}$. By using table 3 the proof is easy. Now we apply formula and do some computation to get our result.

$$Sd(G,x)=\sum_k m(G,k)\times x^{e-k}$$
$$Sd(G,x)=(3n+1)x^{21n+3-(7n+1)}+(3n+1)x^{21n+3-(7n+1)}+3x^{21n+3-(7n+1)}$$
$$\Rightarrow Sd(G,x)=(3n+1)x^{21n+3-7n-1}+(3n+1)x^{21n+3-7n-1}+3x^{21n+3-7n-1}$$
$$\Rightarrow Sd(,x)=(6n+5)^{2(7n+1)}$$

Now we compute PI polynomial of $MC(n)$ nanotube for $n\in\mathbb{N}$. Following theorem shows the PI polynomial for this finite family of nanotubes.

Theorem 2.3.3. Consider the graph of $MC(n)$ nanotube for $n\in\mathbb{N}$. Then its PI polynomial is as follows:

$$PI(G,x)=(42n^2+41n+5)x^{2(7n+1)}$$

Proof. Let G be the graph of $MC(n)$ nanotube for $n\in\mathbb{N}$. The proof of this result is just calculation based. We easily prove it by using table 3. We know that

$$PI(G,x)=\sum_k m(G,k)\times x^{e-k}$$
$$PI(G,x)=(3n+1)(7n+1)x^{21n+3-(7n+1)}+(3n+1)(7n+1)x^{21n+3-(7n+1)}+3(7n+1)x^{21n+3-(7n+1)}$$
$$\Rightarrow PI(G,x)=(21n^2+10n+1)x^{21n+3-7n-1}+(21n^2+10n+1)x^{21n+3-7n-1}+(21n+3)x^{21n+3-7n-1}$$
$$\Rightarrow PI(,x)=(42n^2+41n+5)x^{2(7n+1)}$$

3. Conclusion and general remarks

In this paper, three important counting polynomials called Omega, Sadhana and PI are studied. These polynomials are useful in determining Omega, Sadhana and PI topological indices which play an important role in QSAR/QSPR study. We computed these polynomials for $MLH(k,d)$ nanotube, $CNC_5(n)$ nanocone and $MC(n)$ nanotube.

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