Computing Omega, Sadhana and PI polynomials of benzoid 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. 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, Omega, Sadhana and PI polynomials are computed for Benzoid nanotubes for the first time. The analytical closed formulas of these polynomials for the circumcoronene series of benzenoid H_k, hexagonal parallelogram $P(m,n)$ and zigzag-edge coronoid fused with starphnene $ZCS(k,l,m)$ nanotubes are derived in this paper.

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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 follows:

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

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 $E(G)$, $m(G,k)$ 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. *[4]* 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

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

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.*[6]* 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.*[17]* 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. *[8]* Consider the fullerene graph C_{10n}, $n\geq 10$. Then the Omega and Sadhana polynomials of C_{10n} are computed as follows:

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

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

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

Recently, Imran *et al.* computed the topological indices of of nanostar dendiremers, polyomino chains and interconnection networks[9-14]. 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 of The Circumcoronene series of Benzenoid H_k, Hexagonal Parallelogram $P(m,n)$ and Zigzag-edge Coronoid fused with Starphnene $ZCS(k,l,m)$ nanotubes. For further study of these polynomials their topological indices and polynomials of various nanotubes, consult [3, 9-14, 16]. These polynomials are used to predict various physico-chemical properties of certain chemical compounds.

2.1 The circumcoronene series of benzenoid H_k nanotubes

In this section, we compute Omega, Sadhana and PI polynomials for H_k nanotubes. This nanotube is a trivalent decoration having plane tiling of hexagon. The series H_k plays a special role among hexagonal graphs (alias benzenoid graphs) and is known as the coronene/circumcoronene series. The first term of it is the cycle C_6 which is the molecular graph of the benzene. This family of nanotubes is usually symbolized as H_k. We have $|V(H_k)| = 6k^2$ and $|E(H_k)| = 3(2k + \sum_{r=1}^{k-1} 2(k+r))$.

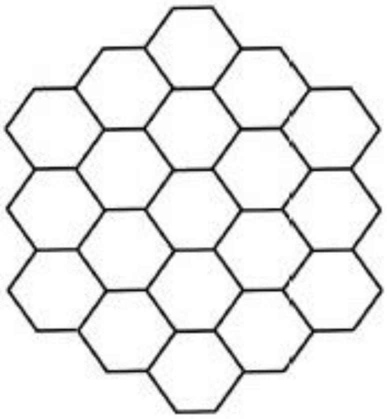

Fig. 1. A representation of H_3 namotube.

Theorem 2.1.1. *The Omega polynomial of H_k nanotube $\forall\ k \in \mathbb{N}$, is as follows:*

$$\Omega(G,x) = 3\{(2k-1) + 2(2k-2)x^{(2k+2(k+1))} + 2(2k-3)x^{(2k+2(k+2))} + \ldots + 2kx^{(2k+2(2k-1))}\}$$

Proof: Let G be the graph of H_k nanotube $\forall\ k \in \mathbb{N}$, Table 1 shows the number of co-distant edges in G. By using Table 1 the proof is mechanical. Now we apply formula and do some calculation to get our result.

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

Table 1. Number of co-distant edges of H_k 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	$2k + \sum_{r=1}^{k-1} 2(k+r)$	$2k - 1 + 2\sum_{r=1}^{k-1}(2k-r-1)$

$$\Omega(G,x) = 3\{(2k-1) + 2\sum_{r=1}^{k-1}(2k-r-1)x^{(2k+\sum_{r=1}^{k-1}2(k+r))}\}$$

$$\Rightarrow \Omega(G,x) = 3\{(2k-1) + 2(2k-1-1)x^{(2k+2(k+1))} + 2(2k-2-1)x^{(2k+2(k+2))} + \ldots + 2(2k-k+1-1)x^{(2k+2(k+k-1))}\}$$

$$\Rightarrow \Omega(G,x) = 3\{(2k-1) + 2(2k-2)x^{(2k+2(k+1))} + 2(2k-3)x^{(2k+2(k+2))} + \ldots + 2kx^{(2k+2(2k-1))}\}$$

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

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

$$Sd(G,x) = 3\{(2k-1) + 2(2k-2)x^{2(2k+2(k+1))} + 2(2k-3)x^{2(2k+2(k+2))} + \ldots 2 + 2kx^{2(2k+2(k+k-1))}\}$$

Proof: Let G be the graph of H_k nanotube $\forall\ k \in \mathbb{N}$. The proof of this result is just calculation based. We prove it by using Table 1. We know that

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

$$Sd(G,x) = 3\{(2k-1) + 2\sum_{r=1}^{k-1}(2k-r-1)x^{2(2k+\sum_{r=1}^{k-1}2(k+r))}\}$$

$$\Rightarrow Sd(G,x) = 3\{(2k-1) + 2(2k-1-1)x^{2(2k+2(k+1))} + 2(2k-2-1)x^{2(2k+2(k+2))} + \ldots 2 + (2k-k+1-1)x^{2(2k+2(k+k-1))}\}$$

$$\Rightarrow Sd(G,x) = 3\{(2k-1) + 2(2k-2)x^{2(2k+2(k+1))} + 2(2k-3)x^{2(2k+2(k+2))} + \ldots 2 + 2kx^{2(2k+2(k+k-1))}\}$$

Next we compute PI polynomial of H_k nanotube. Following theorem explains the PI polynomial of this family of nanotubes.

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

$$PI(G,x) = 3\{(2k(2k-1) + (2k-1)\sum_{r=1}^{k-1}2(k+r) + 4k\sum_{r=1}^{k-1}(2k-r-1) + 2\sum_{r=1}^{k-1}(2k-r-1)(\sum_{r=1}^{k-1}2(k+r)))(x^{2(2k+\sum_{r=1}^{k-1}2(k+r))})\}$$

Proof: Let G be the graph of H_k nanotube $\forall\ k \in \mathbb{N}$. We prove it by using Table 1. We know that

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

$$PI(G,x) = 3\{((2k-1) + 2\sum_{r=1}^{k-1}(2k-r-1))(2k + \sum_{r=1}^{k-1}2(k+r))$$

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

$$\Rightarrow PI(G,x) = 3\{(2k(2k-1) + (2k-1)\sum_{r=1}^{k-1}2(k+r) + 4k\sum_{r=1}^{k-1}(2k-r-1)$$

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

2.2 Hexagonal Parallelogram*P(m, n)* ∀*m, n* ∈ℕ nanotube

In this section, we determine Omega, Sadhana and PI polynomials for $P(m,n)\ \forall\ m,n \in \mathbb{N}$ nanotube. This nanotube have also applied the interpolation method to some other classes of two parametric families of graphs. We just briefly present them for the hexagonal parallelogram graphs $P(m,n)$. These graphs consists of a hexagons arranged is a parallelogram fashion, where the hexagonal parallelogram graph $P(5,4)$ is depicted in figure. In $P(m,n)$ nanotube, where m is the number of hexagons in any row and n is the number of hexagons in any column. We have $|V(P(m,n))| = 2m + 2n + 2mn$ and

$$|E(P(m,n))| = \begin{cases} 2mn + 2m + n + 1 + 2\sum_{i=1}^{m-1}(i+1), & m = n \\ 2mn + m + 2n + 1 + 2\sum_{i=1}^{n}(i+1), & m > n \\ 2mn + 2m + n + 1 + 2\sum_{i=1}^{m}(i+1), & m < n \end{cases}$$

Now we compute Omega polynomial of $P(m,n)$ nanotube.

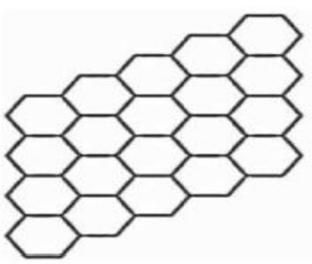

Fig. 2. A representation of P(5,4) nanotube.

Theorem 2.2.1. The Omega polynomial of $P(m,n)$ nanotube $\forall\ m,n \in \mathbb{N}$ is as follows:

$$\Omega(P(m,n),x) = \begin{cases} (n+1)x^{m+1} + mx^{n+1} + 2x^{\sum_{i=1}^{m-1}(i+1)}, m = n \\ nx^{m+1} + (m+1)x^{n+1} + 2x^{\sum_{i=1}^{n1}(i+1)}, m > n \\ (n+1)x^{m+1} + mx^{n+1} + 2x^{\sum_{i=1}^{n}(i+1)}, m < n \end{cases}$$

Proof: Let G be the graph of Hexagonal Parallelogram $P(m,n)\ \forall\ m,n \in \mathbb{N}$ nanotube. Table 2, 3 and 4 shows the number of co-distant edges in G. By using Table 2, 3 and 4 the proof is straightforward.

Table 2. Number of co-distant edges of $P(m,n)$ ∀ $m,n \in \mathbb{N}$ nanotube when m = n

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

Table 3. Number of co-distant edges of $P(m,n)$ ∀ $m,n \in \mathbb{N}$ nanotube when m > n

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

Table 4. Number of co-distant edges of $P(m,n)$ ∀ $m,n \in \mathbb{N}$ nanotube when m < n

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

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 = n

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

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

For $m>n$

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

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

For $m<n$

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

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

In the following theorem, the Sadhana polynomial of Hexagonal Parallelogram $P(m,n)$ $\forall$ m,n $\in\mathbb{N}$ nanotube is computed.

Theorem 2.2.2. The Sadhana polynomial of Hexagonal Parallelogram $P(m,n)$ $\forall$ $m,n\in\mathbb{N}$ nanotube is as follows:

$$Sd(P(m,n),x)=\begin{cases}(n+1)x^{2mn+m+n+2\sum_{i=1}^{m-1}(i+1)}+mx^{2mn+2m+2\sum_{i=1}^{m-1}(i+1)}+\\ 2x^{2mn+2m+n+1+2\sum_{i=1}^{m-1}(i+1)},m=n\\ nx^{2mn+2n+2\sum_{i=1}^{n}(i+1)}+(m+1)x^{2mn+m+n+2\sum_{i=1}^{n}(i+1)}+\\ 2x^{2mn+m+2n+1+\sum_{i=1}^{n}(i+1)},m>n\\ (n+1)x^{2mn+m+n+1+2\sum_{i=1}^{m}(i+1)}+mx^{2mn+2m+2\sum_{i=1}^{m}(i+1)}+\\ 2x^{2mn+2m+n+1+\sum_{i=1}^{m}(i+1)},m<n\end{cases}$$

Proof: Let G be the graph of Hexagonal Parallelogram $P(m,n)$ $\forall$ m,n $\in\mathbb{N}$ nanotube. By using Table 2, 3 and 4, 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 $m=n$

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

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

For $m>n$

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

$$\Rightarrow Sd(G,x)=(n+1)x^{2mn+m+n+1+2\sum_{i=1}^{n}(i+1)}+mx^{2mn+2m+2\sum_{i=1}^{n}(i+1)}+$$
$$2x^{2mn+2m+n+1+\sum_{i=1}^{n}(i+1)}$$

For $m<n$

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

Now we compute PI polynomial of Hexagonal Parallelogram $P(m,n)$ $\forall$ $m,n\in\mathbb{N}$ nanotube. Following theorem shows the PI polynomial for this finite family of nanotubes.

Theorem: Consider the graph of Hexagonal Parallelogram $P(m,n)$ $\forall$ $m,n\in\mathbb{N}$ nanotube. Then its PI polynomial is as follows:

$$PI(P(m,n),x)=\begin{cases}(mn+m+n+1)x^{2mn+m+n+2\sum_{i=1}^{m-1}(i+1)}+(mn+m)x^{2mn+2m+2\sum_{i=1}^{m-1}(i+1)}+\\ 2\sum_{i=1}^{m-1}(i+1)x^{2mn+2m+n+1+\sum_{i=1}^{m-1}(i+1)},m=n\\ (mn+n)x^{2mn+2n+2\sum_{i=1}^{n}(i+1)}+(mn+m+n+1)x^{2mn+m+n+2\sum_{i=1}^{n}(i+1)}+\\ 2\sum_{i=1}^{n}(i+1)x^{2mn+m+2n+1+\sum_{i=1}^{n}(i+1)},m>n\\ (mn+m+n+1)x^{2mn+m+n+2\sum_{i=1}^{m}(i+1)}+(mn+m)x^{2mn+2m+2\sum_{i=1}^{m}(i+1)}+\\ 2\sum_{i=1}^{m}(i+1)x^{2mn+2m+n+1+\sum_{i=1}^{m}(i+1)},m<n\end{cases}$$

Proof: Let G be the graph of Hexagonal Parallelogram $P(m,n)$ $\forall$ m,n $\in\mathbb{N}$ nanotube. The proof of this result is just calculation based. We easily prove it by using Table 2, 3 and 4. We know that

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

For $m = n$

$$PI(G,x) = n(m+1)x^{2mn+2m+n+1+2\sum_{i=1}^{m-1}(i+1)-(m+1)} +$$
$$m(n+1)x^{2mn+2m+n+1+2\sum_{i=1}^{m-1}(i+1)-(n+1)} + 2\sum_{i=1}^{m-1}(i+1)x^{2mn+2m+n+1+2\sum_{i=1}^{m-1}(i+1)-\sum_{i=1}^{m-1}(i+1)}$$
$$+(m+1)x^{2mn+2m+n+1+2\sum_{i=1}^{m-1}(i+1)-(m+1)}$$

$$\Rightarrow PI(G,x) = (mn+m+n+1)x^{2mn+m+n+2\sum_{i=1}^{m-1}(i+1)} +$$
$$(mn+m)x^{2mn+2m+2\sum_{i=1}^{m-1}(i+1)} + 2\sum_{i=1}^{m-1}(i+1)x^{2mn+2m+n+1+\sum_{i=1}^{m-1}(i+1)}$$

For $m > n$

$$PI(G,x) = n(m+1)x^{2mn+m+2n+1+2\sum_{i=1}^{n}(i+1)-(m+1)} +$$
$$m(n+1)x^{2mn+m+2n+1+2\sum_{i=1}^{n}(i+1)-(n+1)} + 2\sum_{i=1}^{n}(i+1)x^{2mn+m+2n+1+2\sum_{i=1}^{n}(i+1)-\sum_{i=1}^{n}(i+1)}$$
$$+(n+1)x^{2mn+m+2n+1+2\sum_{i=1}^{n}(i+1)-(n+1)}$$

$$\Rightarrow PI(G,x) = (mn+n)x^{2mn+2n+2\sum_{i=1}^{n}(i+1)} +$$
$$(mn+m+n+1)x^{2mn+m+n+2\sum_{i=1}^{n}(i+1)} +$$
$$2\sum_{i=1}^{n}(i+1)x^{2mn+m+2n+1+\sum_{i=1}^{n}(i+1)}$$

For $m < n$

$$PI(G,x) = n(m+1)x^{2mn+2m+n+1+2\sum_{i=1}^{m}(i+1)-(m+1)} +$$
$$m(n+1)x^{2mn+2m+n+1+2\sum_{i=1}^{m}(i+1)-(n+1)} + 2\sum_{i=1}^{m}(i+1)x^{2mn+2m+n+1+2\sum_{i=1}^{m}(i+1)-\sum_{i=1}^{m}(i+1)}$$
$$+(m+1)x^{2mn+2m+n+1+2\sum_{i=1}^{m}(i+1)-(m+1)}$$

$$\Rightarrow PI(G,x) = (mn+m+n+1)x^{2mn+m+n+2\sum_{i=1}^{m}(i+1)} +$$
$$(mn+m)x^{2mn+2m+2\sum_{i=1}^{m}(i+1)} + 2\sum_{i=1}^{m}(i+1)x^{2mn+2m+n+1+\sum_{i=1}^{m}(i+1)}$$

2.3 Zigzag-edge Coronoid fused with Starphene nanotubes ZCS(k,l,m)

In this section, we compute Omega, Sadhana and PI polynomials for $ZCS(k,l,m)$ nanotubes. This system considered in this work is a composite benzenoid obtained by fusing a zigzag-edge coronoid $ZC(k,l,m)$ with a starphene $St(k,l,m)$. This system, abbreviated as $ZCS(k,l,m)$, is depicted in figure $ZCS(4,4,4)$. We have $|V(ZCS(k,l,m))| = 36k-54$ and $|E(ZCS(k,l,m))| = 15k+15l+15m-63$. Now we compute Omega polynomial of Zigzag-edge Coronoid fused with Starphene $ZCS(k,l,m)$ nanotube.

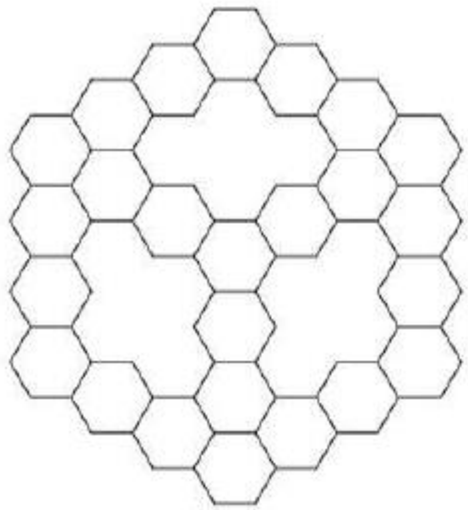

Fig. 3. A representation of $ZCS(4,4,4)$ nanotube.

Theorem 2.3.1. The Omega polynomial of nanotube $ZCS(k,l,m)$ for $k = l = m \geq 4$ is equal to:

$$\Omega(ZCS(k,l,m),x) = (k^2+9)x^{15k-21} + (l^2+9)x^{15l-21} + (m^2+9)x^{15m-21}$$

Proof: Let G be the graph of $ZCS(k,l,m)$ nanotube for $k = l = m \geq 4$. Table 1 shows the number of co-distant edges in G.

By using Table 5 the proof is straightforward.

Table 5. Number of co-distant edges of $ZCS(k,l,m)$ nanotube.

Types of qoc's	Types of edges	No of co-distant edges	No of qoc
C_1	e_1	15k - 21	$k^2 + 9$
C_2	e_2	15l - 21	$l^2 + 9$
C_3	e_3	15m - 21	$m^2 + 9$

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

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

$$\Omega(G,x) = (k^2+9)x^{15k-21} + (l^2+9)x^{15l-21} + (m^2+9)x^{15m-21}$$

In the following theorem, the Sadhana polynomial of

$ZCS(k,l,m)$ nanotube is computed.

Theorem 2.3.2. The Sadhana polynomial of $ZCS(k,l,m)$ nanotube for $k=l=m\geq 4$ is as follows:

$$Sd(G,x)=(k^2+9)x^{15l+15m-42}+(l^2+9)x^{15k+15m-42}+(m^2+9)x^{15k+15l-42}$$

Proof: Let G be the graph $ZCS(k,l,m)$ of nanotube for $k=l=m\geq 4$.By using Table 5 the proof is easy. Now we apply formula and do some computation to get our result.

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

$$Sd(G,x)=(k^2+9)x^{15k+15l+15m-63-15k+21}+(l^2+9)x^{15k+15l+15m-63-15l+21}+$$

$$(m^2+9)x^{15k+15l+15m-63-15m+21}$$

$$\Rightarrow Sd(G,x)=(k^2+9)x^{15l+15m-42}+(l^2+9)x^{15k+15m-42}+(m^2+9)x^{15k+15l-42}$$

Now we compute PI polynomial of $ZCS(k,l,m)$ nanotube for $k=l=m\geq 4$. Following theorem shows the PI polynomial for this finite family of nanotubes.

Theorem 2.3.3. Consider the graph of $ZCS(k,l,m)$ nanotube, for $k=l=m\geq 4$. Then its PI polynomial is as follows:

$$PI(ZCS(k,l,m),x)=(15k^3-21k^2+135k-189)x^{15l+15m-42}+(15l^3-21l^2+135l-189)x^{15k+15m-42}+$$
$$(15m^3-21m^2+135m-189)x^{15k+15l-42}$$

Proof: Let G be the graph of $ZCS(k,l,m)$ nanotube, for $k=l=m\geq 4$. The proof of this result is just calculation based. We easily prove it by using Table 5. We know that

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

$$PI(G,x)=(k^2+9)(15k-21)x^{15k+15l+15m-63-15k+21}+$$
$$(l^2+9)(15l-21)x^{15k+15l+15m-63-15l+21}+$$
$$(m^2+9)(15m-21)x^{15k+15l+15m-63-15m+21}$$

$$\Rightarrow PI(G,x)=(15k^3-21k^2+135k-189)x^{15l+15m-42}$$
$$+(15l^3-21l^2+135l-189)x^{15k+15m-42}$$
$$+(15m^3-21m^2+135m-189)x^{15k+15l-42}$$

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 H_k nanotube, $P(m,n)$ nanotube and $ZCS(k,l,m)$ nanotube.

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References

[1] A. R. Ashrafi, M. Ghorbani, M. Jalali, Indian J. Chem., **47*A***, 535 (2008).
[2] A. Bahrami, J. Yazdani, Digest Journal of Nanomaterials and Biostructures, **3**, 265 (2008).
[3] K. C. Das, F. M. Bhatti, S. G. Lee, I. Gutman, MATCH Commun. Math. Comput. Chem., **65**, 753 (2011).
[4] M. V. Diudea, Omega polynomial, Carpath. J. Math., **22**, 43 (2006).
[5] M. V. Diudea, I. Gutman, J. Lorentz, Molecular Topology, Nova, Huntington2001.
[6] M. V. Diudea, S. Cigher, P. E. John, MATCH Commun. Math. Comput. Chem., **60**, 237 (2008)
[7] M. Ghojavand, A. R. Ashrafi, Digest Journal of Nanomaterials and Biostructures, **3**, 209 (2008).
[8] M. Ghorbani, M. Jalali, Digest Journal of Nanomaterials and Biostructures, **4**, 177 (2009).
[9] S. Hayat, M. Imran, Applied Mathematics and Computation, **240**, 213(2014).
[10] S. Hayat, M. Imran, J. Comput. Theor. Nanosci., Accepted, In press.
[11] S. Hayat, M. Imran, J. Comput. Theor. Nanosci., Accepted, In press.
[12] S. Hayat, M. Imran, J. Comput. Theor. Nanosci., Accepted, In press.
[13] M. Imran, S. Hayat, M. K. Shafiq, Optoelectron. Adv. Mater.-Rapid Comm., **8**(9-10), 948(2014).

[14] M. Imran, S. Hayat, M. Y. H. Malik, Applied Mathematics and Computation, **244**, 936(2014).
[15] B. Rajan, A. William, C. Grigorious, S. Stephen, J. Comp. Math. Sci., **5**, 530 (2012).
[16] I. Tomescu, S. Kanwal, MATCH Commun. Math. Comput. Chem., **69**, 535 (2013).
[17] J. Yazdani, A. Bahrami, Digest Journal of Nanomaterials and Biostructures, **4**, 507(2009).

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