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Research Article

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Closed Form of the Omega and the Sadhana Polynomials of $C_4C_6C_8$ Nanosheet

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ABSTRACT

The counting polynomials are useful in topological description of benzenoid structures. It also helps to describe its topological indices by virtue of quasi-orthogonal cuts of the edge strips in the polycyclic graphs. In this article we give a complete description of the Omega and the Sadhana polynomial of the nanotube $C_4C_6C_8$ and provide its mathematical proof.

Keywords: Nanotubes; Omega Polynomial; Sudhana Polynomial; $C_4C_6C_8$ nanosheet

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INTRODUCTION

A covalent bond is a chemical bond that involves the sharing of electron pairs between atoms. The covalently bonded compounds can be represented as graphs called the molecular graphs. In molecular graphs atoms are viewed as vertices and covalent bonds are viewed as edges between vertices. When we apply the graph theory in the study of molecular graphs it is called chemical graph theory. There are many representations of a graph in chemical graph theory. It includes sequence of numbers, a polynomial, a single number(topological indices), a matrix etc. Each of these representations depicts relevant structural of the underlying molecule.

A structure is a trivalent decoration formed by alternating squares C_4, hexagons C_6 and octagons C_8 is named as C_4 C_6 C_8 $(2n,m)$ nanosheet as shown in Figure 1. The nanosheets are widely used to produce an electrode for a supercapacitor. They have wide range of applications in graphene transistors, solar panels, integrated circuits and many more.

Consider a connected graph $G(V, E)$with the vertex set $V(G)$ and the edge set $E(G)$. Two edges $e = uv$ and $f = xy$ of $E(G)$ are said to be *codistant*, denoted by e *co* f, if they satisfy the following relation:

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

The relation *co* is reflexive as e *co* e always holds for all $e \in E(G)$. Also if e *co* f then f *co* e, thus *co* is also symmetric. The relation *co* is not always transitive. For example for a complete bipartite graph $K_{2,n}$ *co* is not reflexive. If for a graph G the relation *co* is transitive then G is called a *co-graph* and the set of edges $C(e) = \{f \in E(G); f \text{ co } e\}$ is said to be an orthogonal cut *oc* of G. Also then $E(G)$ be a disjoint union of orthogonal cuts i.e. $E(G) = C_1 \cup C_2 \cup \ldots \cup C_k$, $C_i, \cap C_j = \varnothing$, for all $i \neq j$.

The relation *op* between two edges $e = uv$ and $f = xy$ of $E(G)$ holds if e and f are opposite or topologically parallel and is denoted by e *op* f. A set of opposite edges within the same face eventually forming a strip of adjacent faces, termed as an opposite edge strip *ops*, which is a quasi-orthogonal cut *qoc*(i.e., the transitivity relation is not necessarily obeyed). It is to be noted that *co* relation is defined in the whole graph while *op* is defined only in a face. Let $m(G,l)$ be the number of *ops* strips of length l. In [8], the Omega polynomial is defined as

$$\Omega(G,x) = \sum_l m(G,l)x^l$$

Also in [14], the Sadhana polynomial *Sd(G,x)* is defined as

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

Where, $|E(G)|$ is the edge cardinality of the graph. One can obtain the Sadhana polynomial from the definition of the Omega polynomial by replacing l by $|E(G)|-1$ in the exponent. The Omega polynomial has a very strong correlation with the total energy of some molecular structures. These polynomials are widely studied in recent years. For more details see [9], [8], [14], [6], [11], [7], [1], [3], [10], [2] etc.

In this paper, we compute the Omega and the Sadhana polynomials of the nanosheet $C_4\,C_6\,C_8\,(2n,m)$. Throughout the manuscript we use standard notations from [5] and [8].

RESULTS AND DISCUSSION

In this section, we compute the Omega and the Sadhana polynomial of the nanosheet $C_4\,C_6\,C_8\,(2n,m)$, where *2n* is the number of hexagons arrangement row wise and *m* is the number of hexagons arrangements column wise (as shown in the figure). The nanosheet has $|E(C_4\,C_6\,C_8\,(2n,m))| = 15mn - 2n - 3m$. The Omega and the Sadhana polynomials are computed in the following proposition for the nanosheet $C_4\,C_6\,C_8\,(2n,m)$.

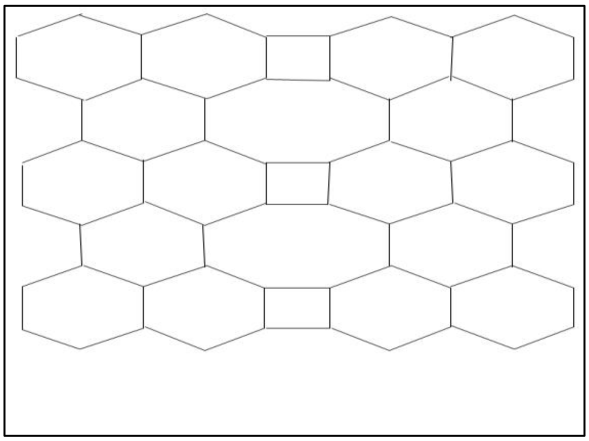

Figure 1: Nanosheet $C_4C_6C_8(4,3)$

Theorem 1 *Let* $G = C_4C_6C_8(2n,m)$ be the graph of the nanosheet. Then the followings holds:

1. **The Omega polynomial of G is given by**

$$\Omega(G,x) = \begin{cases} x^{2n}(mx+m-1)+(n-1)x^{2m}+2(m+n-2)x^{m+n}+4(x^2+x^4+...+x^{2n-2}), & for\ m=n; \\ (mx+m-1)x^{2n}+(5n-2m+1)x^{2m}+4(x^2+x^4+...+x^{2m-2}), & for\ m<n. \\ (mx+m-1)x^{2n}+(n-1)x^{2m}+2(n+k-1)x^{2m+2k-2}+4\sum_{i=1}^{m+k-2}x^{2i}, & for\ m>n\ and\ m-n=k \\ & where\ k=1,2,3,... \\ (mx+m-1)x^{2n}+(n-1)x^{2m}+(n+2k+1)x^{2m}+4\sum_{i=1}^{m-1}x^{2i}, & for\ m>n\ and\ m=2n+k \\ & where\ k=0,1,2,... \end{cases}$$

2. The Sadhana polynomial of G is given by $Sd(G,x) =$

$$\begin{cases} (mx^{2m}+(m-1)x^{3n}+2(m+n-2)x^{2n+m})x^{15mn-5n-5m}+4\sum_{i=1}^{n-1}x^{15mn-2n-3m-2i}, & for\ m=n; \\ (mx^{2m}+(m-1)x^{n+2m}+(5n-2m+1)x^{3n})x^{15mn-5n-5m}+4\sum_{i=1}^{m-1}x^{15mn-2n-3m-2i}, & for\ m<n. \\ (mx^{2m}+(m-1)x^{n+2m}+(n-1)x^{3n})x^{15mn-5n-5m}+2(n+k-1)x^{15mn-2n-5m-2k+2} & \\ +4\sum_{i=1}^{m+k-2}x^{15mn-2n-3m-2i}, & for\ m>n\ and\ m-n=k\ where\ k=1,2,3,\ldots \\ (mx^{2m}+(m-1)x^{n+2m}+(n+2k+1))x^{15mn-5n-5m}+4\sum_{i=1}^{m-1}x^{15mn-2n-3m-2i}, & for\ m>n\ and\ m=2n+k \\ & where\ k=1,2,3,\ldots \end{cases}$$

Proof. Let $G = C_4C_6C_8(2n,m)$ be the graph of the Nanosheet as shown in Figure 1. The graph G has $15mn-2n-3m$ edges. From Figure 1 it is clear that there are four types of qocs. The proof is straight forward from Table 1, 2, 3 and 4.

Table 1: Number of co-distant edges of Nanosheet $C_4C_6C_8(2n,m)$ for $m=n$

Type of qoc	No. of distinct edges	No. of qoc
C_1	$3n$ $2n$	m $m-1$
C_2	$2m$	$n-1$
C_3, C_4	$m+n$ $2i, i=1,2,\ldots,n-1$	$m+n-2$ 2

Therefore, for $m=n$ the Omega polynomial is:

$$\Omega(G,x) = mx^{3n}+(m-1)x^{2n}+(n-1)x^{2m}+2[(m+n-2)x^{m+n}+2\sum_{i=1}^{n-1}x^{2i}]$$
$$= x^{2n}(mx+m-1)+(n-1)x^{2m}+2(m+n-2)x^{m+n}+4(x^2+x^4+\ldots+x^{2n-2})$$

Also, for $m=n$ the Sadhana polynomial is

$$Sd(G,x) = mx^{15n-2n-3m-3n}+(m-1)x^{15mn-2n-3m-2n}+(n-1)x^{15mn-2n-3m-2m}$$
$$+2[(m+n-2)x^{15mn-2n-3m-m-n}+2\sum_{i=1}^{n-1}x^{15mn-2n-3m-2i}]$$
$$= mx^{15mn-5n-3m}+(m-1)x^{15mn-2n-5m}+2(m+n-2)x^{15mn-3n-4m}+4\sum_{i=1}^{n-1}x^{15mn-2n-3m-2i}$$
$$= (mx^{2m}+(m-1)x^{3n}+2(m+n-2)x^{2n+m})x^{15mn-5n-5m}+4\sum_{i=1}^{n-1}x^{15mn-2n-3m-2i}$$

Table 2: Number of co-distant edges of the nanosheet $C_4C_6C_8(2n,m)$ **for** $m<n$

Type of qoc	No. of distinct edges	No. of qoc
C_1	$3n$ $2n$	m $m-1$
C_2	$2m$	$n-1$
C_3,C_4	$2m$ $2i, i=1,2,...,m-1$	$2n-m+1$ 2

From table 2, the Omega polynomial for $m<n$ is equal to

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

$$= x^{2n}(mx+m-1) + x^{2m}(5n-2m+1) + 4(x^2 + x^4 + ... + x^{2m-2}).$$

And for $m<n$ the Sadhana polynomial is given by

$$Sd(G,x) = mx^{15mn-2n-3m-3n} + (m-1)x^{15mn-2n-3m-2n} + (n-1)x^{15mn-2n-3m-2m}$$

$$+ 2[(2n-m+1)x^{15mn-2n-3m-2m} + 2\sum_{i=1}^{m-1} x^{15mn-2n-3m-2i}]$$

$$= mx^{15mn-5n-3m} + (m-1)x^{15mn-4n-3m} + (n-1)x^{15mn-2n-5m} + (4n-2m+2)x^{15mn-2n-5m}$$

$$+ 4\sum_{i=1}^{m-1} x^{15mn-2n-3m-2i}$$

$$= (mx^{2m} + (m-1)x^{n+2m} + (5n-2m+1)x^{3n})x^{15mn-5n-5m} + 4\sum_{i=1}^{m-1} x^{15mn-2n-3m-2i}$$

Table 3: Number of co-distant edges of Nanosheet $C_4C_6C_8(2n,m)$ **for** $m>n \ and \ m-n=k, k=1,2,...$

Type of qoc	no. of distinct edges	No. of qoc
C_1	$3n$ $2n$	m $m-1$
C_2	$2m$	$n-1$
C_3,C_4	$2m+2(k-1)$ $2i, i=1,2,\ldots,m+k-2$	$n+k-1$ 2

From table 3, the Omega polynomial for $m>n$ and $m-n=k, k=1,2,...$ is equal to

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

$$= (mx+m-1)x^{2n} + (n-1)x^{2m} + 2(n+k-1)x^{2m+2k-2} + 4\sum_{i=1}^{m+k-2} x^{2i}.$$

And for $m>n \ and \ m-n=k, k=1,2,...$ the Sadhana polynomial is given by

$$Sd(G,x) = mx^{15n-2n-3m-3n} + (m-1)x^{15mn-2n-3m-2n} + (n-1)x^{15mn-2n-3m-2m}$$
$$+ 2[(n+k-1)x^{15mn-2n-3m-2m-2(k-1)} + 2\sum_{i=1}^{m+k-2} x^{15mn-2n-3m-2i}]$$
$$= mx^{15mn-5n-3m} + (m-1)x^{15mn-4n-3m} + (n-1)x^{15mn-2n-5m}$$
$$+ 2(n+k-1)x^{15mn-2n-5m-2k+2} + 4\sum_{i=1}^{m+k-2} x^{15mn-2n-3m-2i}$$
$$= (mx^{2m} + (m-1)x^{n+2m} + (n-1)x^{3n})x^{15mn-5n-5m}$$
$$+ 2(n+k-1)x^{15mn-2n-5m-2k+2} + 4\sum_{i=1}^{m+k-2} x^{15mn-2n-3m-2i}.$$

Table 4: Number of co-distant edges of Nanosheet $C_4C_6C_8(2n,m)$ **for** $m > n \ and \ m = 2n+k, k = 0,1,2,...$

Type of qoc	No. of distinct edges	No. of qoc
C_1	$3n$ $2n$	m $m-1$
C_2	$2m$	$n-1$
C_3, C_4	$2m$ $2i, i = 1,2,\ldots,m-1$	$k+1$ 2

From table 4, the Omega polynomial for $m > n \ and \ m = 2n+k, k = 0,1,2,...$ is equal to

$$\Omega(G,x) = mx^{3n} + (m-1)x^{2n} + (n-1)x^{2m} + 2[(k+1)x^{2m} + 2\sum_{i=1}^{m-1} x^{2i}]$$
$$= (mx + m - 1)x^{2n} + (n-1)x^{2m} + (n+2k+1)x^{2m} + 4\sum_{i=1}^{m-1} x^{2i}.$$

And for $m > n \ and \ m = 2n+k, k = 0,1,2,...$ the Sadhana polynomial is given by

$$Sd(G,x) = mx^{15n-2n-3m-3n} + (m-1)x^{15mn-2n-3m-2n} + (n-1)x^{15mn-2n-3m-2m}$$
$$+ 2[(k+1)x^{15mn-2n-3m-2m} + 2\sum_{i=1}^{m-1} x^{15mn-2n-3m-2i}]$$
$$= mx^{15mn-5n-3m} + (m-1)x^{15mn-4n-3m} + (n-1)x^{15mn-2n-5m}$$
$$+ 2(k+1)x^{15mn-2n-5m} + 4\sum_{i=1}^{m-1} x^{15mn-2n-3m-2i}$$
$$= (mx^{2m} + (m-1)x^{n+2m} + (n+2k+1))x^{15mn-5n-5m} + 4\sum_{i=1}^{m-1} x^{15mn-2n-3m-2i}.$$

CONCLUSIONS

In this paper, we have calculated the closed form of the Omega and the Sadhana polynomials for the nanosheet $C_4C_6C_8(2n,m)$. These polynomials are useful for calculating topological descriptors(indices) of these structures. These descriptors are also useful in QSAR/QSPR study.

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