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Research Article

Omega, Sadhana, Theta, and PI Polynomials of Double Benzonoid Chain

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Counting polynomials are closely related to certain features of chemical graphs and provide an elegant means of expressing graph topological invariants. The current paper aims to calculate four polynomials for double benzenoid chains, Sadhana, omega, theta, and Padmakar–Ivan (PI). The edge-cut method is used to derive analytical closed expressions for these polynomials.

1. Introduction

In chemistry, graph theory has a wide range of applications, particularly in the mathematical modeling of chemical structures [1–3]. Atoms are referred to as vertices in chemical graph theory, while the bonds that connect them are referred to as edges. Graph $H(V,E)$ is a connected, finite, simple chemical graph, where vertex and edge sets are debited by V and E, respectively. Pólya [4] coined the concept of a counting polynomial in the field of chemistry in 1936. However, chemists did not pay much attention to the subject for several decades, even though characteristic polynomials are computed from molecular orbitals of unsaturated hydrocarbons [5]. Polynomial counting is a common method for expressing molecular invariants in a chemical graph in polynomial form. Chemical graph features such as equidistant edges, independent sets, matching sets, and chromatic numbers influence these polynomials. Characteristic polynomials, Hosoya polynomial, rotational polynomial, Wiener polynomial, and sextet polynomial are some well-known polynomials. Polynomials can be used to produce a variety of significant topological indices, either directly or thenceforth integrals or derivatives. A topological index is a numeric quantity that can quantify many chemical properties in organic chemistry and is invariant under the graph's automorphism and derived according to specific rules. Topological indices were first used in chemistry in 1947; Harary Wiener introduced a renowned topological descriptor called the Wiener index [6], which is given as

$$W(H) = \frac{1}{2} \sum_{p \in V(G)} \sum_{q \in V(G)} d(p,q), \tag{1}$$

where $d(p,q)$ is the shortest distance between vertices p and q.

For a molecular graph $H(V,E)$, the edges $e = xy$ and $f = wz$ of H are called codistant, denoted by $eCof$ if they satisfy the following topologically parallel relation: $d(x,z) = d(y,w) = d(x,w) + 1 = d(y,z) + 1$ and. $d(x,w) = d(y,z)$.

Co is symmetric and reflexive. It is not transitive in general. Set $C(e) = \{f \in E(G)\colon eCof\}$. The given relation "*Co*" is transitive on $C(e)$, and $C(e)$ is said to be orthogonal cut *oc* in the graph. It is named a quasiorthogonal cut *qoc* if the relation *Co* is not transitive.

By quasiorthogonal cuts, omega, theta, PI polynomials, and Sadhana are well-defined. Diudea [7] defined omega polynomial $\Omega(H,x)$ as calculating "quasiorthogonal cut" strips, qoc strips in H as

$$\Omega(H,t) = \sum_k m(H,k)t^k, \quad (2)$$

where $m(H, k)$ represents the number of qoc of length k.

Diudea et al. [8] were the first to introduce the theta polynomial $\theta(H, x)$ in 2008. It is defined as counting several edges equidistant for each edge f of the graph and given as

$$\theta(H,t) = \sum_k m(H,k)kt^k. \quad (3)$$

The Sadhana polynomial denoted by $s\,d(H, t)$ was introduced by Ashrafi et al. [9]. It is given as follows:

$$\mathrm{sd}(H,t) = \sum_k m(H,k)t^{e-k}. \quad (4)$$

After Khadikar et al. [10] presented the Padmakar–Ivan (PI) index, Ashrafi et al. [11] proposed the PI polynomial. The polynomial, denoted by PI(H, t), counts no equidistant edges in G and is given as follows:

$$\mathrm{PI}(H,t) = \sum_k m(H,k)kt^{e-k}. \quad (5)$$

Counting polynomials have piqued the interest of analysts and researchers working in the field of chemical graph theory, with some recent work included in [12–16]. In addition, various topological features of hexagonal chains have been considered in [17–20]. This paper calculated four counting polynomials of double benzenoid chains: Sadhana, omega, theta, and Padmakar–Ivan (PI).

2. Results and Discussion

2.1. Counting Polynomials and a Double Benzenoid Hexagonal Chain. Benzenoid hydrocarbons play a significant role in organic chemistry. This hexagonal system has congruent interior regions and contains no cut vertex. The system is named pericondensed if at least one vertex belongs to three hexagons; otherwise, the hexagonal system is said to be catacondensed. The chain is an arrangement of hexagons in which no two hexagons are adjacent to each other. We obtain n-tuple hexagonal chain which is formed when condensed identical hexagonal chains combine [9, 21].

A double hexagonal chain can be obtained when $n=2$ [22, 23]. A pericondensed hexagonal system is formed with the aid of a new fused naphthalene, which is a double hexagonal (benzenoid) chain.

Let us have a look at the naphthalene structure with horizontal internal edges. There are two types of naphthalene fusion in this regard, as shown in Figure 1.

$$\begin{aligned} &\alpha-\text{type}: v=1,\ w=2,\ x=3,\ y=4, \\ &\beta-\text{type}: u=2, v=3,\ w=4,\ x=\ 5. \end{aligned} \quad (6)$$

At every stage, fusion type is obtained by η, where $\eta \in \{\alpha, \beta\}$. A double (benzenoid) chain is denoted by $H(\eta_1, \eta_2, \ldots, \eta_n)$ where $\eta_1, \eta_2, \ldots, \eta_n \in \{\alpha, \beta\}$ are fusion types, respectively. It is seen that $H(\eta_1, \eta_2, \ldots, \eta_n)$ contains $2n+2$ regular hexagons and $n+1$ naphthalene, see Figure 1. The number of codistant edges of the double benzenoid chain $H(\alpha, \beta, \alpha, \beta, \ldots, \alpha, \beta)$ is given in Table 1.

The details of double hexagonal (benzenoid) chains can be seen in [21, 24–27]. The edge-cut procedure proposed by Klavzar [28] will be used to compute the counting polynomials.

Theorem 1. *The omega polynomial of the double hexagonal* $H_{(\alpha,\beta,\alpha,\beta,\ldots,\beta)}$ *is given by*

$$\Omega(H(\alpha,\beta,\alpha,\beta,\ldots,\beta),t) = 2t^2 + 2t^4 + (n+2)t^3 + (n-2)t^5. \quad (7)$$

Proof. Consider a graph H of a double hexagonal chain $H(\alpha,\beta,\alpha,\beta,\ldots,\beta)$, with $8n+11$ number of edges. The omega polynomial of graph H is $\Omega(H,t) = \sum_k m(H,k)t^k$.

The elementary cuts of the double benzenoid hexagonal chain are described in Figure 2.

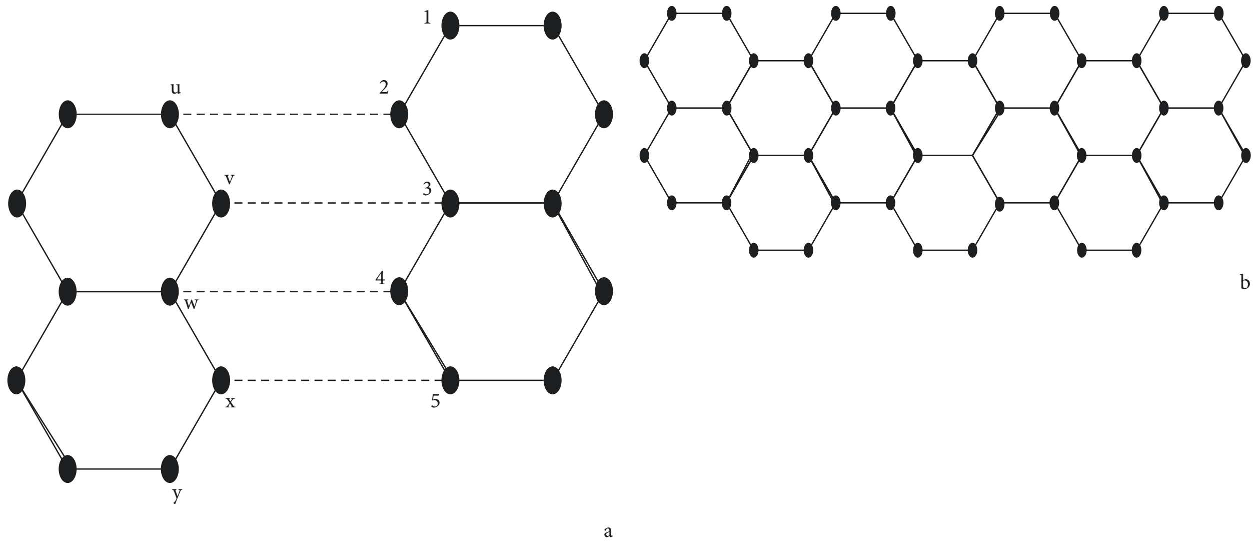
Using Table 1 for the number of qocs and the number of codistant edges, we get the desired result.

$$\Omega(H(\alpha,\beta,\alpha,\beta,\ldots,\beta),t) = 2t^2 + 2t^4 + (n+3)t^3 + (n-2)t^5. \quad (8)$$

□

Theorem 2. *The Sadhana polynomial of the double hexagonal* $H(\alpha,\beta,\alpha,\beta,\ldots,\alpha,\beta)$ *is given by*

$$\mathrm{sd}(H(\alpha,\beta,\alpha,\beta,\ldots,\beta),t) = t^{8n+6}\left(2t^3 + (n+3)t^2 + 2t + n-2\right). \quad (9)$$



(a) (b)

Figure 1: (a) Naphthalene fusion β type in the double hexagonal benzenoid chain. (b) A double hexagonal benzenoid chain $H(\eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6)$.

Table 1: Number of codistant edges of the double benzenoid hexagonal chain $H(\alpha, \beta, \alpha, \beta, \ldots, \alpha, \beta)$ (using Figure 2).

Types of qocs	Types of edges	No. of codistant edges	No. of qocs
		2	2
M	s_1	4	2
		5	$n-2$
S	s_2	3	$n+3$

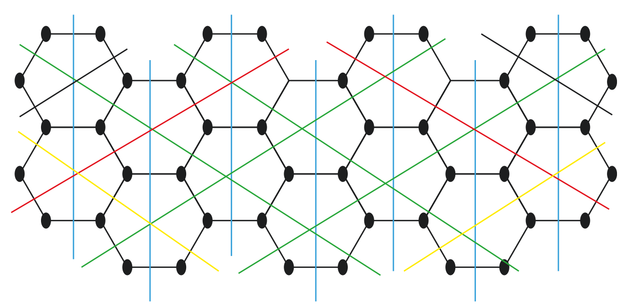


Figure 2: The elementary cuts of the double benzenoid hexagonal chain $H(\alpha, \beta, \alpha, \beta, \alpha, \beta)$.

Proof. Consider a graph H of a double hexagonal chain $H(\alpha, \beta, \alpha, \beta, \ldots, \beta)$. The Sadhana polynomial of graph H is $s\,d(H, t) = \sum_k m(H, k) t^{e-k}$, where $e = |E| = 8n + 11$.

Using Table 1 for the number of qocs and the number of codistant edges, we get the desired result.

$$\mathrm{Sd}(H(\alpha, \beta, \alpha, \beta, \ldots, \beta), t) = (n-2)t^{8n+11-5} + (n+3)t^{8n+11-3} + 2t^{8n+11-4} + 2t^{8n+11-2}. \tag{10}$$

On simplifying it becomes

$$\mathrm{Sd}(H(\alpha, \beta, \alpha, \beta, \ldots, \beta), t) = t^{8n+6}\left(2t^3 + (n+3)t^2 + 2t + n - 2\right). \tag{11}$$

□

Theorem 3. *The theta polynomial of the double hexagonal* $H(\alpha, \beta, \alpha, \beta, \ldots, \alpha, \beta)$ *is given by*

$$\theta(H(\alpha, \beta, \alpha, \beta, \ldots, \beta), t) = 4t^2 + 8t^4 + 3(n+3)t^3 + 5(n-2)t^5. \quad (12)$$

Proof. Consider a graph H of a double hexagonal chain $H(\alpha, \beta, \alpha, \beta, \ldots, \beta)$. The theta polynomial of graph H is

$$\theta(H, t) = \sum_k m(H, k)kt^k. \quad (13)$$

Using Table 1 for several qocs and several codistant edges, we get the desired result.

$$\theta(H(\alpha, \beta, \alpha, \beta, \ldots, \beta), t) = 4t^2 + 8t^4 + 3(n+3)t^3 + 5(n-2)t^5. \quad (14)$$

□

Theorem 4. *The PI polynomial of the double hexagonal* $H(\alpha, \beta, \alpha, \beta, \ldots, \alpha, \beta)$ *is given by*

$$\mathrm{PI}(H(\alpha, \beta, \alpha, \beta, \ldots, \beta), t) = t^{8n+6}\left(4t^3 + 3(n+3)t^2 + 8t + 5n - 10\right). \quad (15)$$

Proof. Consider a graph H of a double hexagonal chain $H(\alpha, \beta, \alpha, \beta, \ldots, \beta, \alpha)$. The PI polynomial of graph H with $e = |E| = 8n + 3$ is $\mathrm{PI}(H, t) = \sum_k m(H, k)kt^{e-k}$.

Using Table 1 for the number of qocs and the number of codistant edges, we get

$$\mathrm{PI}(H(\alpha, \beta, \alpha, \beta, \ldots, \beta, \alpha), t) = 5(n-2)t^{8n+11-5} + 3(n+3)t^{8n+11-3} + 8t^{8n+11-4} + 4t^{8n+11-2}. \quad (16)$$

On simplifying, we get

$$\mathrm{PI}(H(\alpha, \beta, \alpha, \beta, \ldots, \beta, \alpha), t) = t^{8n+6}\left(4t^3 + 3(n+3)t^2 + 8t + 5n - 10\right). \quad (17)$$

□

2.2. Double Benzenoid Hexagonal Linear Chain and Counting Polynomials. $H(\eta_1, \eta_2, \ldots, \eta_n)$ is said to be a double linear hexagonal (benzenoid) chain, $L_{2\times n}$, if for all i, $\eta_i = \eta_{i+1}$ in $H(\eta_1, \eta_2, \ldots, \eta_n)$, see Figure 3. $L_{2\times n}$ has $8n + 11$ edges. The number of codistant edges of the double benzenoid chain $L_{2\times n}$ is given in Table 2.

Theorem 5. *The omega polynomial of the double hexagonal* $L_{2\times n}$ *is given by*

$$\Omega(L_{2\times n}, t) = 2t^{n+2} + (2n+1)t^3 + 2t^2. \quad (18)$$

Proof. Consider the double hexagonal chain $L_{2\times n}$ and omega polynomial of the graph H as

$$\Omega(H, t) = \sum_k m(H, k)t^k. \quad (19)$$

The elementary cuts of the double benzenoid linear chain are described in Figure 4.

Using the definition of omega polynomial, and putting the values of $m(H, k)$ and k from Table 2, we get the desired result that

$$\Omega(L_{2\times n}, t) = 2t^{n+2} + (2n+1)t^3 + 2t^2. \quad (20)$$

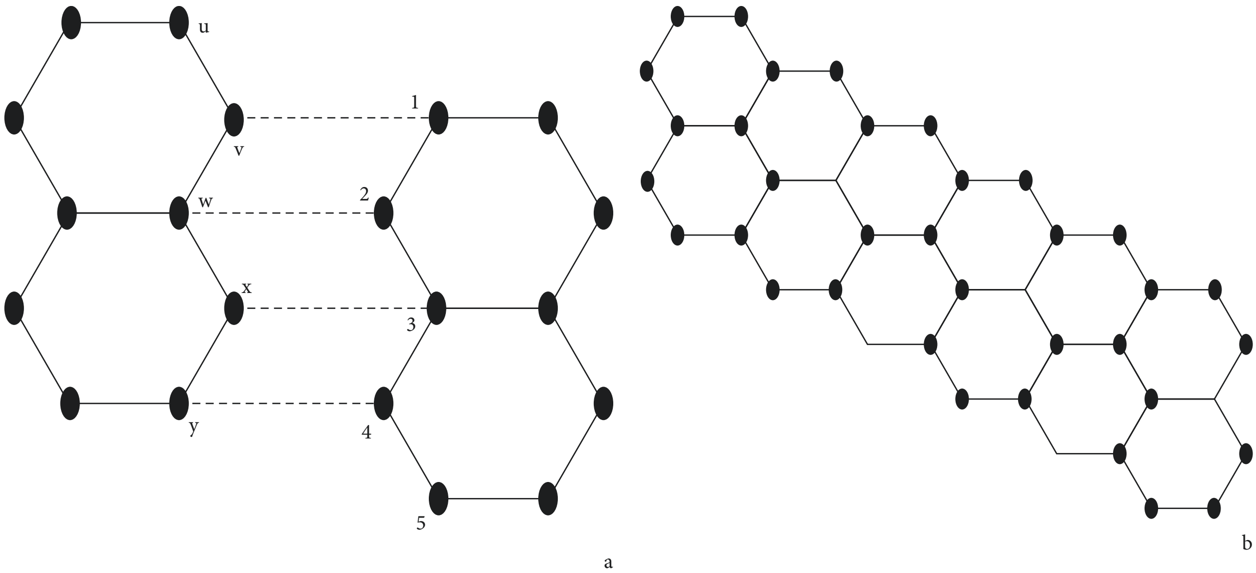
□

Theorem 6. *The Sadhana polynomial of the double linear hexagonal* $L_{2\times n}$ *is given as follows:*

$$\mathrm{Sd}(L_{2\times n}, t) = t^{7n+8}\left(2t^{n+1} + (2n+1)t^n + 2t\right). \quad (21)$$

Proof. Since $\mathrm{sd}(H, t) = \sum_k m(H, k)t^{e-k}$, $e = 8n + 11$.

Again using Table 2, and putting the values of $m(H, k)$ and k in the definition of Sadhana polynomial, we get



(a) (b)

Figure 3: (a) Naphthalene α type fusion in the double hexagonal benzenoid chain. (b) A double linear hexagonal benzenoid chain $L_{2\times 5}$.

Table 2: Number of codistant edges of the double linear benzenoid chain $L_{2\times n}$.

Types of qocs	Types of edges	No. of codistant edges	No. of qocs
M	s_1	$n+2$	2
N	s_2	3	$2n+1$
N	s_2	2	2

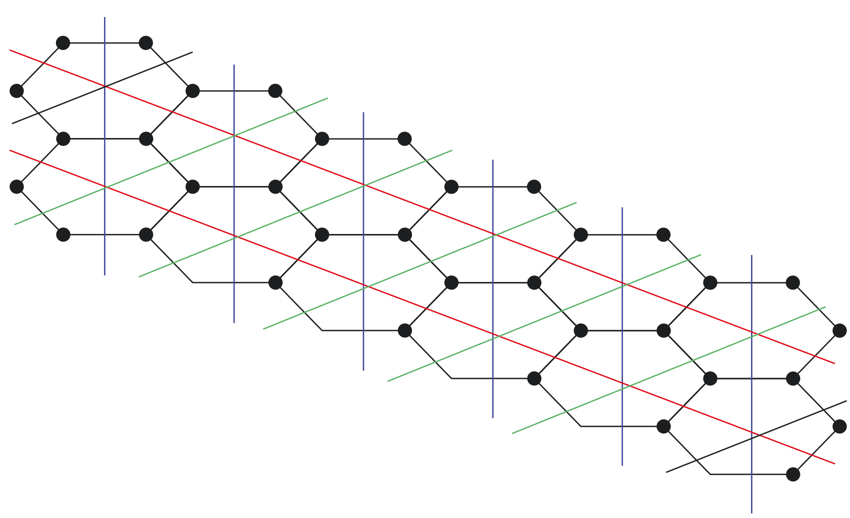


Figure 4: The elementary cuts of the double benzenoid linear chain $L_{2\times 5}$.

$$\mathrm{Sd}\left(L_{2\times n},t\right) = 2t^{8n+11-n-2} + (2n+1)t^{8n+11-3} + 2t^{8n+11-2}. \tag{22}$$

On simplifying, we get

$$\mathrm{Sd}\left(L_{2\times n},t\right) = t^{7n+8}\left(2t^{n+1} + (2n+1)t^{n} + 2t\right). \tag{23}$$

□

Theorem 7. *The theta polynomial of the double linear hexagonal $L_{2\times n}$ is given by*

$$\theta\left(L_{2\times n},t\right) = (2n+4)t^{n+2} + (6n+3)t^{3} + 4t^{2}. \tag{24}$$

Proof. We know that $\theta(H,t) = \sum_k m(H,k)kt^k$.

Putting values of $m(H,k)$ and k from Table 1, we get

$$\theta\left(L_{2\times n},t\right) = 2(n+2)t^{n+2} + 3(2n+1)t^{3} + 4t^{2}, \tag{25}$$

which simplifies to

$$\theta\left(L_{2\times n}, t\right) = (2n+4)t^{n+2} + (6n+3)t^{3} + 4t^{2}. \tag{26}$$

□

Theorem 8. *The PI polynomial of the double linear hexagonal $L_{2\times n}$ is given by*

$$\mathrm{PI}\left(L_{2\times n}, t\right) = t^{7n+8}\left(4t^{n+1} + (6n+3)t^{n} + (4n+2)t\right). \tag{27}$$

Proof. By definition, PI polynomial is given as $e = |E| = 8n + 11$ and

$$\mathrm{PI}\left(L_{2\times n}, t\right) = \sum_{k} m(H,k)kt^{e-k}. \tag{28}$$

Again employing Table 2 for values of k and $m(H,k)$, we get the following polynomial:

$$\mathrm{PI}\left(L_{2\times n}, t\right) = 2(n+2)t^{8n+11-n-2} + 3(2n+1)t^{8n+11-3} + 4t^{8n+11-2}, \tag{29}$$

which leads the result.

$$\mathrm{PI}\left(L_{2\times n}, t\right) = t^{7n+8}\left(4t^{n+1} + (6n+3)t^{n} + (2n+4)t\right). \tag{30}$$

□

3. Conclusion

Counting polynomials are a simple technique to encode topological indices of chemical graphs, which are quantifiers of various physiochemical aspects of compounds and are commonly employed in structure-activity correlations. The edge-cut method of Klavzar is used to compute distance-based counting polynomials of the double benzenoid chain, such as omega, Sadhana, theta and PI polynomials. These polynomials are well-known methods for matching the chemical graph with the physiological features of various double benzenoid chains.

Data Availability

All data are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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