Research Article

Wei Gao, Saad Ihsan Butt, Muhammad Numan, Adnan Aslam*, Zeeshan Malik, Muhammad Waqas

Omega and the related counting polynomials of some chemical structures

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Abstract: Counting polynomials are mathematical functions having as coefficients the multiplicity of property partition and as exponent the extent of the corresponding partition. In this work, four counting polynomials are computed: omega, theta, sadhana, and Padmakar–Ivan (PI) polynomials of benzene ring embedded in the P-type surface on 2-D network and n-phenylene. Moreover, the closed formulas of the corresponding indices of these polynomials are also proposed. These results could help to better understand the topology of these important structures.

Keywords: omega-type polynomials, benzene ring embedded in P-type surface, n-phenylene

1 Introduction

Graph theory has found many application in chemistry, especially in mathematical modeling of the chemical structures [1–3]. In chemical graph theory, we often model a chemical structure by a graph, where the atoms correspond to the vertices and bonds to the edges between them. A graph $H$ is an ordered pair $(V(H), E(H))$, where $V(H)$ is the set of vertices and $E(H)$ is the set of edges. The degree of any vertex $u$ is denoted by $d_u$ and is defined as the cardinality of set of neighbors of $u$. A path $P_k$ is the graph with vertex set $V(P_k) = \{v_0, v_1, \ldots, v_{k-1}, v_k\}$ and the edge set $E(P_k) = \{v_0v_1, v_1v_2, \ldots, v_{k-1}v_k\}$. The distance between two vertices $u$ and $v$, denoted by $d(u, v)$ is the length of the shortest path between them. For undefined terminologies and notations, we refer the reader to [4].

The idea of counting polynomial was first introduced by Polya [5] in 1936. This concept received a little attention from chemists for a long time. However, the spectra of the characteristic polynomial of graphs were studied extensively by numerical means to find the molecular orbitals of unsaturated hydrocarbons [6]. In quantum chemistry, the levels of $\pi$ electron energy in conjugated hydrocarbons can be computed by using Hückel theory, as a root of characteristic polynomial [7,8]:

$$P(H, x) = \det[xI - A(H)]$$

(1)

where $A(H)$ is the adjacency matrix of graph $H$ and $I$ is a unit matrix of order equal to the order of $H$. The characteristic polynomial is involved in the evaluation of the topological effect on molecular orbitals, topological resonance energy, the aromatic sextet theory, the Kekulé structure count, etc. [8–10]. The above equation can be written in a simplified form:

$$P(H, x) = \sum_k \eta(H, k)x^k$$

(2)

For a graph $H$, the coefficients $\eta(H, k)$ of the polynomial can be calculated by using Sachs graphs, which are subgraphs of $H$. Equation (2) was independently established by Sachs, Harary, Milic, Spialter, Hosoya, etc. [11]. The extension of relation 1 was made by Hosaya [12] and others [13–15] by replacing the adjacency matrix of $H$ with distance matrix and next by any square topological matrix. The general form of counting polynomial is given
in Equation (2), where the exponent shows the extent of partition \( P_H \cup P_H = P_H \) of a graph property \( P_H \) and the coefficients \( m(H, k) \) are related to the occurrence of partitions of extent \( k \). In mathematical chemistry, counting polynomials are related with Hosoya [16,17]; independent edge sets are counted by \( Z(H, x) \) and distances counted by \( \mathcal{H}(H, x) \) polynomials [18,19]. Their roots and coefficients are used for the characterization of topological nature of hydrocarbons. Hosoya also proposed the sextet polynomial [20–22] for counting the resonant rings in a benzenoid molecule.

In this article, we will compute four counting polynomials, namely, omega, theta, sadhana and Padmakar–Ivan (PI) polynomials of benzene ring embedded in P-type surface on 2-D network and \( n \)-phenylene. Before giving the formal definition of these counting polynomials, we need to define few basic concepts related to graph theory. Let \( H(V, E) \) be a planar bipartite graph. Two edges \( f = u_1u_2 \) and \( g = v_1v_2 \) are co-distant (briefly \( fco\ g \)) to each other if

\[
d(u_1, v_1) = d(u_2, v_2)
\]

and

\[
d(u_2, v_1) = d(u_1, v_2) + 1 = d(u_2, v_2) + 1.
\]

The relation \( co \) is reflexive and symmetric but in general it is not transitive. For instance, in the complete bipartite graph \( K_{3,3} \), the relation \( co \) is not transitive. If the relation \( co \) is transitive, then we call the graph co-graph. Let \( C(f) = \{g \in E(H) : g \ co \ f\} \) be the set of all edges of \( G \) which are co-distant to the edge \( f \in E(H) \). The set \( C(f) \) is called orthogonal cut of \( G \) with respect to edge \( f \). If the co is an equivalence relation, then the set \( E(G) \) is the union of disjoint orthogonal cuts; \( E(H) = C_1 \cup C_2 \cup \cdots \cup C_k \) and \( C_i \cap C_j = \emptyset \), \( i \neq j \).

A subgraph \( K \subset H \) is called isometric if \( d_H(u, v) = d_E(u, v) \) for any two vertices \( u, v \in E(H) \). Also, \( H \) is convex if for any \( u, v \in V(K) \), the shortest path between \( u \) and \( v \) in \( H \) is in \( K \). In a planar graph \( H \), two edges \( f \) and \( g \) are in relation opposite, denoted by \( fop\ g \), if they are the opposite edges of an inner face of \( H \). The relation \( fco\ g \) follows from the fact that the faces are isometric. Note that the relation \( op \) is defined only in faces. The relation \( op \) partitions the edges set of \( G \) into opposite edge strip ops. In general, the transitivity does not hold for the relations ops and qoc (quasi-orthogonal cuts).

Let \( \eta(H, k) \) be the number of qoc strips of length \( k \). The omega polynomial \( \Omega(H, x) \) of a graph \( G \) was introduced by Diudea [23] and is defined as

\[
\Omega(H, x) = \sum_{k} \eta(H, k) \times x^k
\]

The theta polynomial \( \Theta(H, x) \) was introduced by Diudea [24] in 2008. It counts the number of edges equidistant to every edge \( f \) of \( G \) and is defined as

\[
\Theta(H, x) = \sum_{k} \eta(H, k) k \times x^k
\]

The \( \prod(H, x) \) polynomial introduces by Diudea [24] counts the edges nonequidistant to the reference edges \( f \) and is defined as

\[
\prod(H, x) = \sum_{k} \eta(H, k) k \times x^{f-k}
\]

Sadhana polynomial denoted by \( sd(H, x) \) is related to ops of a graph \( G \) and counts the nonopposite edges in \( G \). It was introduced by Ashrafy et al. [25,26] and is defined as

\[
sd(H, x) = \sum_{k} \eta(H, k) \times x^{f-k}
\]

The first derivative of these counting polynomials computed at \( x = 1 \) gives information on counting topological property:

\[
\Omega'(H, x)|_{x=1} = \sum_{k} k \times \eta(H, k) = f = E(H)
\]

\[
\Theta'(H, x)|_{x=1} = \Theta(H) = \sum_{k} k^2 \times \eta(H, k)
\]

\[
\prod'(H, x)|_{x=1} = \Pi(H) = \sum_{k} k \times (f - k) \times \eta(H, k)
\]

\[
sd'(H, x)|_{x=1} = sd(H) = \sum_{k} (f - k) \times \eta(H, k).
\]

From the Equations (7) and (8), one can compute \( PI(G) \) as follows:

\[
PI(H) = f^2 - \sum_{k} k^2 \times \eta(H, k) = (\Omega(H, x)|_{x=1})^2
\]

\[
- \Theta(H, x)|_{x=1}
\]

Also, the Cluj–Ilmenau index [27], denoted by \( CI(H) \), can be computed from omega polynomial as:

\[
CI(H) = (\Omega(H, x)|_{x=1})^2 - \Omega(H, x)|_{x=1} - \Omega'(H, x)|_{x=1}
\]

The omega counting polynomial is proved to be useful in description of polyhedral coverings appearing in nanostructures [28]. The topological descriptor \( CI \) has found utility in predicting the stability of small fullerenes as well as the resonance energy of planar benzenoids. Omega polynomial is also useful in describing the topology of tubular nanostructures. For more details of
the computation of counting polynomial and topological
indices, see ref. [29–37].

2 Omega-type polynomials of benzene ring embedded in P-type surface in 2D network

O’Keeffe et al. [38] proposed a structure of benzene ring embedded in P-type surface which contains only one kind of carbon atoms. In these structures, six- and eight-membered rings occur in 2:3 ratio, and its primitive unit cell contains only 24 atoms. This structure is stable, comparable with C_{60} and can be described as a three-dimensional linkage of C_{8} rings. In this section, we are computing the omega-type polynomials of benzene ring embedded in P-type surface on 2D network. Let P(m, n) denote the molecular structure of benzene ring embedded in P-type surface on 2D network, where m and n are the numbers of unit cells in each column and row, respectively. The graph of P(m, n) is shown in Figure 1. It is easy to observe that P(m, n) contains 24mn vertices and 32mn − 2m − 2n edges. In the next theorem, we will compute the omega-type counting polynomials of P(m, n).

**Theorem 1.** Let m, n ∈ ℤ, then the omega, theta, sadhana and ∏ polynomials of P(m, n) are equal to:

1. \( \Omega(P(m, n), x) = 12x^{2mn} + (2m - 1)x^{2m} + (2n - 1)x^{2n} \)
2. \( \theta(P(m, n), x) = 24mnx^{2mn} + 2m(2m - 1)x^{2m} + 2n(2n - 1)x^{2n} \)
3. \( \prod(P(m, n), x) = 24mnx^{30mn - 2m - 2n} + 2(n(2m - 1)x^{32mn - 2m - 2n} - 1) ) \)
4. \( \text{Sd}(P(m, n), x) = 12x^{30mn - 2m - 2n} + (2m - 1)x^{32mn - 2m - 4n} + (2n - 1)x^{32mn - 4m - 2n} \)

**Proof.** To compute these omega-type polynomials of P(m, n), we need to find the quasi-orthogonal cuts (qocs) and count the number of edges used in the qocs. One unit cell of P(m, n) contains eight types of qocs as it is shown in Figures 2 and 3. We can generalize these quasi-orthogonal cuts to the whole graph. The total number of these cuts and the total edges used in these cuts are presented in Table 1. Now using the values from Table 1
in the definition of omega, theta, ∏ and sadhana polynomial, we get the required result.

From the above theorem, it is easy to see that

\[ \Omega(P[m, n], 1) = 12 \times 2mn + (2m - 1) \times (2n) + (2n - 1) \times (2m) \]
\[ = 32mn - 2m - 2n = |E(P[m, n])| \]
\[ \theta(P[m, n]) = 48m^2n^2 + 4n^2(2m - 1) + 4m^2(2n - 1) \]
\[ = 8mn(6mn + m + n) - 4(m^2 + n^2). \]
\[ Sd(P[m, n]) = 12(30mn - 2m - 2n) + (2m - 1)(32mn - 2m - 4n) + (2n - 1)(32mn - 4m - 2n) \]
\[ = 8mn(8m + 8n + 35) - 18(m + n) - 4(m^2 + n^2). \]

### 3 Omega-type polynomials of cyclic \( n \) phenylene

Analogous to catacondensed benzenoids, Berris et al. [39] introduced \( n \)-phenylenes, where \( n \) is the number of benzene rings. In \( n \) phenylenes, benzene rings are separated by a square called cyclobutadiene. Pericondensed benzenoids do not have analogous \( n \) phenylenes, but the catacondensed chain may close on itself to form a super-ring. Figure 4 depicts cyclic 4 phenylene.
we compute the omega-type polynomial and the corresponding topological indices of \( n \)-phenylenes. It is easy to do that since the numbers of vertices and edges of \( n \)-phenylenes are \( 6n \) and \( 8n \), respectively. For simplicity, we denote the molecular graph of \( n \)-phenylenes by \( R_n \).

**Theorem 2.** Let \( n \geq 3 \), then the omega, theta, \( \prod \) and sadhana polynomials of \( R_n \) are equal to

1. \( \Omega(R_n, x) = 2nx^4 \)
2. \( \theta(R_n, x) = 8nx^3 \)
3. \( \prod(R_n, x) = 8nx^{8n-4} \)
4. \( \text{Sd}(R_n, x) = 2nx^{8n-4} \).

**Proof.** We use the idea of orthogonal cuts to count the number of equidistance edges. There are two types of orthogonal cuts in \( R_n \). They are denoted by \( C_1 \) and \( C_2 \) as it is shown in Figure 5. The \( C_1 \) and \( C_2 \) orthogonal cuts cover all edges of \( R_n \). The total number of quasi-orthogonal cuts and total number of edges in these quasi-orthogonal cuts are presented in Table 2. Using the values from Table 2 in the definition of omega, theta, \( \prod \) and sadhana polynomials, we get the required results. \( \square \)

From the above theorem, it is easy to see that

\[
\Omega(R_n, 1) = 4 \times 2n = 8n = |E(R_n)|.
\]

\[
\theta(R_n) = 8n \times n = 8n^2.
\]

\[
\text{Sd}(R_n) = 2n(8n - 4) = 16n^2 - 8n.
\]

The topological index \( \text{PI}(R_n) \) can be computed by using Equation (11):

\[
\text{PI}(R_n) = (8n)^2 - (32n) = 64n^2 - 32n.
\]

Finally, the Cluj–Ilmenau index can be computed by using Equation (12) as follows:

\[
\text{Cl}(R_n) = (8n)^2 - 8n - 24n = 64n^2 - 32n.
\]

## 4 Conclusion

Omega and theta polynomials count the equidistant edges in a graph \( H \), while PI polynomial counts nonequidistant ones. In this article, we computed omega, theta, \( \prod \) and sadhana polynomials of benzene ring embedded in P-type surface in 2D network and cyclic \( n \) phenylene. Furthermore, the exact expressions for the topological indices associated with these polynomials have been computed.

**Conflict of interest:** The authors hereby declare that there is no conflict of interests regarding the publication of this article.

**Ethical approval:** The conducted research is not related to either human or animal use.

**Data availability statement:** No data are required for this study.
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