Counting Polynomials of Benzenoid Systems

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Abstract—

The Omega polynomial \( \Omega(G,x) \) for counting qoc strips in \( G \) is defined as 
\[
\Omega(G,x) = \sum_c m(G,c)x^c
\]
with \( m(G,c) \) being the number of strips of length \( c \). Other three related polynomials can be calculated on ops as 
\[
\Theta(G,x) = \sum_c m(G,c)c.x^c
\]
\[
SD(G,x) = \sum_c m(G,c)x^{\lfloor |E(G)|/c \rfloor} - c
\]
\[
\Theta(G,x) = \sum_c m(G,c)c.x^{\lfloor |E(G)|/c \rfloor} - c
\]
and \( \Omega(G,x), \Theta(G,x) \) and \( \Pi(G,x) \) polynomials most important in some physic-chemical structures of molecules. In this paper, these above polynomials and their indices of a class of Benzenoid system are determined.

Key Words—Molecular graph; Benzenoid system, qoc strip, Omega polynomial, Sadhana polynomial, Theta polynomial, Pi polynomial

I. INTRODUCTION

Let \( G=(V,E) \) be a simple connected graph with the vertex set \( V=V(G) \) and the edge set \( E=E(G) \), without loops and multiple edges. Two edges \( e=uv \) and \( f=xy \) of \( G \) are called co-distant (briefly: \( e \; co \; f \)) if they obey the topologically parallel edges relation. For some edges of a connected graph \( G \) there are the following relations satisfied [1-3]:

\[
e \; co \; e \\
e \; co \; f \iff f \; co \; e \\
e \; co \; f \; & \; f \; co \; h \rightarrow eco \; h
\]

though the last relation is not always valid. Set \( C(e) = \{ f \in E(G) | f \; co \; e \} \). If the relation “co” is transitive on \( C(e) \) then \( C(e) \) is called an orthogonal cut “oc” of the graph \( G \). The graph \( G \) is called “co-graph” if and only if the edge set \( E(G) \) is the union of disjoint orthogonal cuts.

Let \( m(G,c) \) be the number of qoc strips of length \( c \) (i.e., the number of cut-off edges) in the graph \( G \). Four counting polynomials have been defined [3-23] on the ground of qoc strips:

\[
\Omega(G,x) = \sum_c m(G,c)x^c
\]
\[
\Theta(G,x) = \sum_c m(G,c)c.x^c
\]
\[
SD(G,x) = \sum_c m(G,c)x^{\lfloor |E(G)|/c \rfloor} - c
\]
\[
\Theta(G,x) = \sum_c m(G,c)c.x^{\lfloor |E(G)|/c \rfloor} - c
\]

The summations runs up to the maximum length of qoc strips in \( G \). \( \Omega(G,x) \) and \( \Theta(G,x) \) polynomials count “equidistant edges” in \( G \) while \( SD(G,x) \) and \( \Pi(G,x) \), “non-equidistant edges”. The first derivative (computed at \( x=1 \)) of these counting polynomials provide interesting topological indices:

\[
\Omega'(G,1) = \sum_c m(G,c) \times c
\]
\[
\Theta'(G,1) = \sum_c m(G,c) \times c^2
\]
\[
SD'(G,1) = \sum_c m(G,c) \times \lfloor |E(G)|/c \rfloor - c
\]
\[
\Pi'(G,1) = \sum_c m(G,c) \times c \times \lfloor |E(G)|/c \rfloor - c\times |E(G)|\times c - \Theta(G)
\]

Of course, first derivative of omega polynomial (in \( x=1 \)), equals the number of edges in the graph \( G \). If \( G \) is bipartite, then a qoc starts and ends out of \( G \) and so \( \Omega(G,1) = r/2 \), in which \( r \) is the number of edges in out of \( G \).

The Omega polynomial \( \Omega(G,x) \) for counting qoc strips in \( G \) was defined by M.V. Diudea. Also the Sadhana index \( SD(G) \) was defined by Khadikar et.al. [24,25].
From above equations, one can obtain the Sadhana polynomial and Pi polynomial by replacing $x^i$ with $x^{[E_i]}$ in Omega polynomial and Theta polynomial.

Herein, our notation is standard and taken from the standard book of graph theory [26]. The aim of this study is to compute these counting polynomials of a class of Benzenoid system and called hexagonal system $B_{m,n}$. Reader can see general representation of this family in Figure 1.

![Fig. 1. A general representation of the Benzenoid system $B_{a,b}$ ($\forall a,b \geq 1$).](image)

II. MAIN RESULTS AND DISCUSSION

The aim of this section is to compute the Theta and Pi polynomials of an infinite class of benzenoid system $B_{m,n}$ ($\forall m,n \in \mathbb{N}$) with $4ab+4a+2b-2$ vertices/atoms and $6ab+5a+b-4$ edges/bonds. A general representation of this benzenoid system is shown in Figure 1.

**Theorem 1.** [18] Consider the molecular graph of benzenoids $B_{m,n}$ ($\forall m,n \in \mathbb{N}$) then

If $a \geq b+2$: 
$$\Omega(B_{a,b}, x) = (b+1)x^a + bx^{a+1} + \sum_{i=1}^{b} (4x^{2i-1}) + 2(a-b-1)x^{2b+2}$$

If $a \leq b+1$:
$$\Omega(B_{a,b}, x) = (b+1)x^a + bx^{a+1} + \sum_{i=1}^{a-1} (4x^{2i-1}) + 2(b-a+1)x^{2a}$$

**Theorem 2:** [19] The Sadhana polynomial of hexagonal system $B_{m,n}$ is equal to

- $a \geq b+2, Sd(B_{a,b}, x) = (b+1)x^{E(B_{a,b})}-2a + bx^{E(B_{a,b})}-a-1 + 4\sum_{i=1}^{b} x^{E(B_{a,b})}-2i+1 + 2(a-b-1)x^{E(B_{a,b})}-2b-2$
- $a \leq b+1, Sd(B_{a,b}, x) = (b+1)x^{E(B_{a,b})}-2a + bx^{E(B_{a,b})}-a-1 + 4\sum_{i=1}^{a-1} x^{E(B_{a,b})}-2i+1 + 2(b-a+1)x^{E(B_{a,b})}-2a$

Then the Sadhana index of $B_{m,n}$ is

- $a \geq b+2, Sd(B_{a,b})=12a^2b+24ab^2+10a^3+14ab-2b^2-16a-14b+6$
- $a \leq b+1, Sd(B_{a,b})=12a^2b+24ab^2+10a^2+10ab+4b^2-18a-18b+8$

**Theorem 3.** Consider the benzenoid system $B_{m,n}$ ($\forall m,n \in \mathbb{N}$); the Theta polynomial of $B_{m,n}$ is calculated by formulas:

- $a \geq b+2, \Theta(B_{a,b}, x) = a(b+1)x^a + b(a+1)x^{a+1} + 4\sum_{i=1}^{b} (2i+1)x^{2i+1} + 2(2b+2)(a-b-1)x^{2b+2}$
- $a \leq b+1, \Theta(B_{a,b}, x) = a(b+1)x^a + b(a+1)x^{a+1} + 4\sum_{i=1}^{a-1} (2i+1)x^{2i+1} + 4a(b-a+1)x^{2a}$

Then the Theta index of $B_{m,n}$ is
\[ \forall a \geq b + 2, \ \vartheta(B_{a,b}) = -\frac{8b^3}{3} - 8b^2 + 8ab^2 + 2a^2b - 14ab + 24b + a^2 + 8a - 8 \]

\[ \forall a \geq b + 1, \ \vartheta(B_{a,b}) = \frac{16b^3}{3} + 16b^2 + \frac{35b^2}{3} + 10a^2b + 2ab + 8a^3 + 9a^2 \]

**Theorem 4.** The Pi polynomial \( \Pi(B_{a,b}, x) \) and Pi index \( \Pi(B_{a,b}) \) are equal to

\[ \forall a \geq b + 2, \ \Pi(B_{a,b}, x) = a(b + 1)x^{-a} + b(a + 1)x^{-a-1} + 4\sum_{i=1}^{b} (2i + 1)x^{-2i-1} + 4(b + 1)(a - b - 1)x^{-2b-2} \]

\[ \forall a \geq b + 1, \ \Pi(B_{a,b}, x) = a(b + 1)x^{-a} + b(a + 1)x^{-a-1} + 4\sum_{i=1}^{b} (2i + 1)x^{-2i-1} + 4(a - b + 1)x^{-2a} \]

Then \( \Pi(B_{a,b}) \) is

\[ \forall a \geq b + 2, \ \Pi(B_{a,b}) = 36a^2b^2 + \frac{8b^3}{3} + 9b^2 + 4ab^2 + 58a^2b - 24ab + 24a^2 - 32b - 48a + 24 \]

\[ \forall a \leq b + 1, \ \Pi(B_{a,b}) = 36a^2b^2 - \frac{16b^3}{3} - 15b^2 - 8a^3 + 50a^2b + 12ab^2 + 16a^2 - 40ab - 40a - \frac{59b}{3} + 16 \]

**Proof of Theorem 3.** Let \( G = B_{a,b} \) be the hexagonal system, with \( 4ab + 4a + 2b + 2 \) vertices. To compute the counting polynomials of \( G \), it is enough to calculate \( C(e) \) for every \( e \) in \( E(G) \). By using the Cut Method and from Figures 2, one can see that there are two types of edges-cut of hexagonal system. We denote the corresponding edges-cut by \( C_i \) and \( C_{j} \). By Table 1 and Table 2 we have

<table>
<thead>
<tr>
<th>quasi-orthogonal cuts</th>
<th>Number of co-distant edges</th>
<th>No.</th>
</tr>
</thead>
<tbody>
<tr>
<td>( C_{2i+1} ) ( \forall i = 0, \ldots, b )</td>
<td>1</td>
<td>( a )</td>
</tr>
<tr>
<td>( C_{2i} ) ( \forall i = 1, \ldots, b )</td>
<td>1</td>
<td>( a + 1 )</td>
</tr>
<tr>
<td>( C_{i} ) ( \forall i = 1, \ldots, b )</td>
<td>4</td>
<td>( 2i + 1 )</td>
</tr>
<tr>
<td>( C_{b+1} )</td>
<td>2(a-b-1)</td>
<td>( 2b+2 )</td>
</tr>
</tbody>
</table>

\[ \forall a \geq b + 2: \ \vartheta(B_{a,b}, x) = \sum_{c} m(B_{a,b}, c) . x^c \]

\[ = a(b + 1)x^{b} + b(a + 1)x^{b+1} + 4\sum_{i=1}^{b} (2i + 1)x^{2i+1} + 2(b + 2)(a - b - 1)x^{2b+2} \]

\[ \forall a \leq b + 1: \ \vartheta(B_{a,b}, x) = a(b + 1)x^{b} + b(a + 1)x^{b+1} + 4\sum_{i=1}^{a-1} (2i + 1)x^{2i+1} + 4(a - b + 1)x^{2a} \]

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</thead>
<tbody>
<tr>
<td>( C_{2i+1} ) ( \forall i = 0, \ldots, b )</td>
<td>1</td>
<td>( a )</td>
</tr>
<tr>
<td>( C_{2i} ) ( \forall i = 1, \ldots, b )</td>
<td>1</td>
<td>( a + 1 )</td>
</tr>
<tr>
<td>( C_{i} ) ( \forall i = 1, \ldots, a-1 )</td>
<td>4</td>
<td>( 2i + 1 )</td>
</tr>
<tr>
<td>( C_{a} )</td>
<td>2(b-a+1)</td>
<td>( 2a )</td>
</tr>
</tbody>
</table>

and this completes the proof.\( \blacksquare \)
Fig. 2. The presentation of quasi-orthogonal cuts (qoc strips) of $B_{a,b}$.

Therefore, $\forall a \geq b + 2$:

$$\Theta'(B_{a,b}, x)|_{x=1} = \frac{\partial}{\partial x} \left( a(b+1)x^0 + b(a+1)x^a + 4 \sum_{i=1}^{b} (2i+1)x^{2i+1} + 2(2b+2)(a-b-1)x^{2b+2} \right) |_{x=1}$$

$$= a^2(b+1) + b(a+1)^2 + 4b \sum_{i=1}^{b} (2i+1)^2 + 8(a-b-1)(b+1)^2$$

$$= a^2(b+1) + b(a+1)^2 + 4\left( \sum_{i=1}^{b} 4i^2 \right) + 4b \sum_{i=1}^{b} 4i + 8(-b^3 + b^2(a-3) - b(2a-3) + a - 1)$$

$$= -\frac{8b^3}{3} - 8b^2 + 8ab^2 + 2a^2b - 14ab + 24b + a^2 + 8a - 8$$

And also $\forall a \leq b + 1$:

$$\Theta'(B_{a,b}, x)|_{x=1} = \frac{\partial}{\partial x} \left( a(b+1)x^0 + b(a+1)x^a + 4 \sum_{i=1}^{a} (2i+1)x^{2i+1} + 4a(b-a+1)x^{2a} \right) |_{x=1}$$

$$= a^2(b+1) + b(a+1)^2 + 4\sum_{i=1}^{b} (2i+1)^2 + 8a^2(b-a+1)$$

$$= \frac{16b^3}{3} + 16b^2 + \frac{35b}{3} + 2a^2b + 2ab + a^2 + 8a^2 - 8a^3 + 8a^2$$

$$= \frac{16b^3}{3} + 16b^2 + \frac{35b}{3} + 10a^2b + 2ab + 8a^3 + 9a^2$$

Here the proof is completed. ■

Proof of Theorem 4. Let $G=B_{a,b}$ be the hexagonal system, the proof is analogous to the proof of Theorem 3. By Table 1 and Table 2, the Pi polynomial $\Pi(B_{m,n}, x)$ is equal to $\forall a \geq b + 2$:

$$\Pi(B_{a,b}, x) = \sum_{e} m(B_{a,b}, C_e) C_e x^{E(B_{a,b})}$$

$$= \sum_{i=0}^{b} m(B_{a,b}, C_{2i+1}) C_{2i+1} x^{v_{2i+1}} + \sum_{i=0}^{b} m(B_{a,b}, C_{2i+1}) C_{2i+1} x^{v_{2i+1}} + \sum_{i=0}^{b} m(B_{a,b}, C) C_{2i+1} x^{v_{2i+1}} + m(B_{a,b}, C) C_{2i+1} x^{v_{2i+1}}$$
\[ a(b+1)x^{e-a} + b(a+1)x^{e-a-1} + \sum_{i=1}^{b} (2i+1)x^{e-2i-1} + 4(b+1)(a-b-1)x^{e-2b-2} \]

Where \( e = |E(B_{a,b})| = 6ab + 5a + b - 4 \)

\( \forall a \leq b+1: \Pi(B_{a,b}, x) = a(b+1)x^{e-a} + b(a+1)x^{e-a-1} + \sum_{i=1}^{b} (2i+1)x^{e-2i-1} + 4(b+1)(a-b-1)x^{e-2b-2} \)

By definition of \( \Pi(G) \) index, one can obtain the following computations.

\( \forall a \geq b + 2: \Pi(B_{a,b}, x) = \Pi(B_{b,a}, x) \bigg|_{x=1} \)

\[ \frac{\partial}{\partial x} \left( a(b+1)x^{e-a} + b(a+1)x^{e-a-1} + \sum_{i=1}^{b} (2i+1)x^{e-2i-1} + 4(b+1)(a-b-1)x^{e-2b-2} \right) \bigg|_{x=1} \]

\[ = \left( 36a^2b^2 + 25a^2 + b^2 + 16 \right) + 60a^2b + 12ab^2 - 48ab + 10ab - 40a - 8b \]

\[ = \left( -8b^3 - 8b^2 + 8ab^2 + 2a^2 b - 14ab + 24b + a^2 + 8a - 8 \right) \]

\[ = 36a^2b^2 + 8b^3 + 9b^2 + 4ab^2 + 58a^2b - 24ab + 24a^2 - 32b - 48a + 24 \]

\( \forall a \leq b+1: \Pi(B_{a,b}, x) = \Pi(B_{b,a}, x) \bigg|_{x=1} \)

\[ \frac{\partial}{\partial x} \left( a(b+1)x^{e-a} + b(a+1)x^{e-a-1} + \sum_{i=1}^{b} (2i+1)x^{e-2i-1} + 4(b+1)(a-b-1)x^{e-2b-2} \right) \bigg|_{x=1} \]

\[ = 36a^2b^2 - \frac{16b^3}{3} - 8a^3 + 50a^2b + 12ab^2 - 15b^2 + 16a^2 - 40ab - 40a - \frac{50b}{3} + 16 \]

These complete the proof.■

### III. Conclusion

In this paper, we obtained the Omega \( \Omega(G,x) \), Sadhana \( Sd(G,x) \), Theete \( \Theta(G,x) \) and Pi \( \Pi(G,x) \) polynomials and their indices of molecular graph hexagonal system \( B_{a,b} \) for the first time.

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### References


