Hosoya and Harary Polynomials of Hourglass and Rhombic Benzenoid Systems

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In the fields of chemical graph theory, topological index is a type of a molecular descriptor that is calculated based on the graph of a chemical compound. In 1947, Harry Wiener introduced "path number" which is now known as Wiener index and is the oldest topological index related to molecular branching. Hosoya polynomial plays a vital role in determining Wiener index. In this report, we compute the Hosoya polynomials for hourglass and rhombic benzenoid systems and recover Wiener and hyper-Wiener indices from them.

1. Introduction

Cheminformatics is a new branch of science which relates chemistry, mathematics, and computer sciences. Quantitative structure-activity (QSAR) and structure-property relationships (QSPR) are the main components of cheminformatics which are helpful to study physicochemical properties of chemical compounds [1–3].

A topological index is a numeric quantity associated with a graph which characterizes the topology of graph and is invariant under graph automorphism [4–8]. There are numerous applications of graph theory in the field of structural chemistry. The first well-known use of a topological index in chemistry was by Wiener in the study of paraffin boiling points [9]. After that, in order to explain physicochemical properties, various topological indices have been introduced.

The Hosoya polynomial of a graph is a generating function about distance distribution, introduced by Haruo Hosoya in 1988 [10]. This polynomial has many chemical applications [11]; in particular, Wiener index can be directly obtained from the polynomial and studied extensively [12–14].

The Wiener index was first introduced by Harold Wiener in 1947 to study the boiling points of paraffin [9]. It plays an important role in the so-called inverse structure-property relationship problems [15]. For more details about this topological polynomial and index, see the paper series and the references therein [16–20]. In this report, we study Hosoya polynomials, Wiener index, and hyper-Wiener index of hourglass and rhombic benzenoid systems.

2. Preliminaries

Definition 1 (simple graph). A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of $G$ called edges.
Definition 2 (Hosoya polynomial [10]). The Hosoya polynomial of a connected graph $G$ is denoted by $H(G, x)$ and defined as follows:

$$H(G, x) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} x^{d(v, u)},$$

(1)

where $d(u, v)$ denotes the distance between vertices $u$ and $v$.

Definition 3 (Wiener index [9]). The Wiener index of a connected graph $G$ is denoted by $W(G)$ and defined as the sum of distances between all pairs of vertices in $G$, i.e., it can be formulated as follows:

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} d(u, v).$$

(2)

Note that the first derivative of the Hosoya polynomial at $x = 1$ is equal to the Wiener index:

$$W(G) = \frac{\partial H(G)}{\partial x}\bigg|_{x=1}.$$ 

(3)

Definition 4 (modified Wiener index). The modified Wiener index of a connected graph $G$ is denoted by $W_{\lambda}(G)$ and defined as the sum of $\lambda$ power distances between all pairs of vertices in $G$, where $\lambda = 1, 2, 3, 4, \ldots$ i.e., it can be formulated as follows:

$$W(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} d(u, v)^{\lambda}.$$ 

(4)

For detailed survey about this index, see [21–23].

Definition 5 (hyper-Wiener index). Hyper-Wiener index is another distance-based graph invariants used for predicting physicochemical properties of organic compounds [24]. The hyper-Wiener index was introduced by Randić [25] as follows:

$$WW(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} \left( d(u, v) + d(u, v)^2 \right).$$

(5)

Definition 6 (modified hyper-Wiener index). Modified hyper-Wiener index (see [26, 27]) of a connected graph $G$ is denoted by $WW_{\lambda}(G)$ and defined as follows:

$$WW_{\lambda}(G) = \frac{1}{2} \sum_{v \in V(G)} \sum_{u \in V(G)} \left( d(u, v)^{\lambda} + d(u, v)^{2\lambda} \right),$$

(6)

where $\lambda = 1, 2, 3, 4, \ldots$.

Definition 7 (Harary polynomial). The Harary polynomial (see [28, 29]) of a connected graph $G$ is denoted by $h(G)$ and defined as follows:

$$h(G) = \sum_{v \in V(G)} \sum_{u \in V(G)} \frac{1}{d(v, u)^{t}} x^{d(v, u)}.$$ 

(7)

Definition 8 (generalized Harary index). The generalized Harary index (see [30, 31]) of a connected graph $G$ is denoted by $h_t(G)$ and defined as follows:

$$h_t(G) = \sum_{v \in V(G)} \sum_{u \in V(G)} \frac{1}{d(v, u)^{t}} + t,$$

(8)

where $t = 1, 2, 3, 4, \ldots$.

Definition 9 (multiplicative Wiener index). The multiplicative wiener index (see [32, 33]) of a connected graph $G$ is denoted by $\pi(G)$ and defined as follows:

$$\pi(G) = \prod_{u, v \in V(G)} d(u, v).$$

(9)

For detailed applications of topological indices in chemistry, we refer [34–41] and the references therein.

3. Methodology

To compute the Hosoya polynomial of a graph $G$, we need to compute number of pairs of vertices at distance 1, 2, 3, $\ldots$, dia$(G)$, where dia$(G) = \max\{d(u, v) : u, v \in V(G)\}$. For this purpose, we use mathematical induction. Here, the dia$(X_n) = 4n - 1$ and dia$(R_n) = 2n + 1$. The general view of Hosoya polynomial is as below, where $d$ is the diameter of graph:

$$H(G; x) = a_0(n)x^0 + a_1(n)x^1 + a_2(n)x^2 + \cdots + a_d(n)x^d.$$ 

(10)

4. Computational Results

Benzenoid hydrocarbons play a vital role in our environment and in the food and chemical industries. Benzenoid molecular graphs are systems with deleted hydrogens. It is a connected geometric figure obtained by arranging congruent regular hexagons in a plane, so that two hexagons are either disjoint or have a common edge. This figure divides the plane into one infinite (external) region and a number of finite (internal) regions. All internal regions must be regular hexagons. Benzenoid systems are of considerable importance in theoretical chemistry because they are the natural graph representation of benzenoid hydrocarbons. A vertex of a hexagonal system belongs to, at most, three hexagons. A vertex shared by three hexagons is called an internal vertex.

Definition 10 (benzenoid hourglass system). Let $X_n$ denotes the benzenoid hourglass, which is obtained from two copies of a triangular benzenoid $T_n$ by overlapping their external hexagons (Figure 1).

4.1. Results for Benzenoid Hourglass System. The benzenoid hourglass system has $2(n^2 + 4n - 2)$ vertices and $3n^2 + 9n - 6$ edges.
Theorem 1. For the benzenoid hourglass system $X_n$, we have

$$H(X_n; x) = 2(n^2 + 4n - 2) + (3n^2 + 9n - 6) + (6n^2 + 12n - 12)x^2$$

$$+ \sum_{m=1 \mod (2), 1 < m \leq 2n} \left( \frac{19m^3}{24} - 3m^2n - 5m^2 + 3mn^2 + 12mn + \frac{221m}{24} - 17 \right)x^m$$

$$+ \sum_{m=0 \mod (2), 1 < m \leq 2n} \left( \frac{19m^3}{24} - 3m^2n - 5m^2 + 3mn^2 + 12mn + \frac{59m}{6} - 20 \right)x^m$$

$$+ \sum_{m=0 \mod (2), 2 < m \leq 2n-2} \left( \frac{m^3}{24} - \frac{m^2n}{4} + \frac{mn^2}{2} + \frac{n^3}{3} - m^2 + 4n^2 - \frac{35m}{6} + \frac{23n}{3} - 4 \right)x^{2n+m}$$

$$+ \sum_{m=1 \mod (2), 3 < m \leq 2n-2} \left( \frac{m^3}{24} - \frac{m^2n}{4} + \frac{mn^2}{2} + \frac{n^3}{3} - m^2 + 4n^2 - \frac{143m}{24} - \frac{n^3}{12} + \frac{101n}{12} - 5 \right)x^{2n+m}$$

$$+ \left( \frac{133n}{6} + \frac{11(n-1)^2}{2} + \frac{(n-1)^3}{3} - \frac{127}{6} \right)x^{2n+1} + (n^2 + 2)x^{4n-1}.$$  \hspace{1cm} (11)

**Proof.** To prove this theorem, we need to compute $|a_m(n)|$ where $m = 1, 2, 3, \ldots, 4n - 1$. It is easy to verify that

$$|a_0(n)| = |V| = 2(n^2 + 4n - 2),$$

$$|a_1(n)| = |E| = 3n^2 + 9n - 6, \hspace{1cm} (12)$$

$$|a_2(n)| = 6n^2 + 12n - 12.$$  \hspace{1cm}

The remaining proof is divided into six parts which are according to the parity of $m$. \hfill \Box

**Case 1.** $m \equiv 1 \mod (2)$, $1 < m \leq 2n$.

It can be observed from Figure 1 that

$$|a_3(1)| = 0,$$

$$|a_3(2)| = 41,$$

$$|a_3(3)| = 95,$$  \hspace{1cm} (13)

$$|a_3(4)| = 167,$$

$$|a_3(5)| = 257.$$  \hspace{1cm}

Now, one can conclude that

$$|a_3(n)| = 9(n-1)^2 + 27(n-1) + 5. \hspace{1cm} (14)$$  

Using a similar fashion, we have
\[|a_5(1)| = 0,\]
\[|a_5(2)| = 0,\]
\[|a_5(3)| = 93,\]
\[|a_5(4)| = 183,\]
\[|a_5(5)| = 303,\]
\[|a_5(6)| = 453.\]  
(15)

It implies that
\[|a_5(n)| = 15(n - 2)^2 + 45(n - 2) + 33.\]  
(16)

In a similar fashion, we infer
\[|a_6(n)| = 21(n - 3)^2 + 63(n - 3) + 74,\]
\[|a_6(n)| = 27(n - 4)^2 + 81(n - 4) + 130,\]
\[|a_{11}(n)| = 33(n - 5)^2 + 99(n - 5) + 203,\]
\[\cdots.\]  
(17)

In terms of mathematical induction, we yield
\[|a_m(n)| = 3m\left(n - \frac{m}{2} + \frac{1}{2}\right)^2 + 9m\left(n - \frac{m}{2} + \frac{1}{2}\right)\]
\[+ \frac{9((m/2) - (1/2))^2 + ((m/2) - (1/2))^3}{2} + \frac{217 + 73m}{12},\]
\[|a_m(n)| = \frac{19m^2}{24} - 3m^2n - 5m^2 + 3mn^2 + 12nm + \frac{221m}{24} - 17.\]  
(18)

**Case 2.** \(m \equiv 0 \text{mod}(2), 2 < m \leq 2n.\)

It can be observed from Figure 1 that
\[|a_4(1)| = 0,\]
\[|a_4(2)| = 38,\]
\[|a_4(3)| = 98,\]
\[|a_4(4)| = 182,\]
\[|a_4(5)| = 290.\]  
(19)

Now, one can conclude that
\[|a_4(n)| = 12(n - 1)^2 + 24(n - 1) + 2.\]  
(20)

By means of the same trick, we obtain
\[|a_6(1)| = 0,\]
\[|a_6(2)| = 0,\]
\[|a_6(3)| = 84,\]
\[|a_6(4)| = 174,\]
\[|a_6(5)| = 300,\]
\[|a_6(6)| = 462,\]  
(21)

which reveals that
\[|a_6(n)| = 18(n - 2)^2 + 36(n - 2) + 30.\]  
(22)

In light of the similar approach, we get
\[|a_8(n)| = 24(n - 3)^2 + 48(n - 3) + 72,\]
\[|a_{10}(n)| = 30(n - 4)^2 + 60(n - 4) + 130,\]
\[|a_{12}(n)| = 36(n - 5)^2 + 72(n - 5) + 206,\]
\[\cdots.\]  
(23)

Hence, by mathematical induction, we have
\[|a_{19}(n)| = \frac{19m^3}{24} - 3m^2n - 5m^2 + 3mn^2 + 12nm + \frac{59m}{6} - 20.\]  
(24)

**Case 3.** \(m \equiv 1 \text{mod}(2), 3 \leq m \leq 2n - 2.\)

It can be observed from Figure 1 that
\[|a_5(1)| = 0,\]
\[|a_5(2)| = 0,\]
\[|a_5(3)| = 44,\]
\[|a_{11}(4)| = 41,\]
\[|a_{11}(5)| = 101,\]
\[|a_{11}(6)| = 177,\]
\[|a_{11}(7)| = 274.\]  
(25)

Now, one can conclude that
\[|a_{2n-1}(n)| = \frac{(n - 2)^3}{3} + \frac{15}{2}(n - 2)^2 + \frac{193}{6}(n - 2) + 4.\]  
(26)

Using a similar fashion, we have
\[|a_6(1)| = 0,\]
\[|a_6(2)| = 0,\]
\[|a_6(3)| = 0,\]
\[|a_{11}(4)| = 0,\]
\[|a_{11}(5)| = 101,\]
\[|a_{11}(6)| = 150,\]
\[|a_{11}(7)| = 254,\]
\[|a_{11}(8)| = 383,\]
\[|a_{21}(9)| = 539.\]  
(27)

It implies that
In terms of mathematical induction, we yield
\[
\begin{align*}
[a_{2n+1}(n)] &= \left( \frac{(n-(m+1)/2)^3}{3} + \frac{1}{2} \left( \frac{m}{2} - 1 \right) + 11 \right) \\
&\quad \times \left( \frac{n-(m+1)}{2} \right)^2 + \frac{1}{6} \left( \frac{12(m-1)}{2} \right)^2 \\
&\quad + \frac{72(m-1)}{2} + 109 \frac{n-(m+1)}{2} \\
&\quad \times \left( \frac{m^2}{2} + 2 \frac{m-1}{2} + 1 \right), \\
[a_{2n+1}(n)] &= \frac{m^3}{24} - \frac{m^2 n}{4} - \frac{m^2}{2} + \frac{mn^2}{2} - \frac{143m}{24} + \frac{n^3}{3} \\
&\quad + 4n^3 + \frac{101n}{12} - 5.
\end{align*}
\]

(30)

Case 4. \( m \equiv 0 \mod (2), 2 \leq m \leq 2n - 2. \)

It can be observed from Figure 1 that
\[
\begin{align*}
[a_1(1)] &= 0, \\
[a_6(2)] &= 16, \\
[a_7(3)] &= 108, \\
[a_{10}(4)] &= 41, \\
[a_{12}(5)] &= 180, \\
[a_{14}(6)] &= 272, \\
[a_{16}(7)] &= 386.
\end{align*}
\]

(31)

Case 5. \( m = 2n + 1. \)

It can be observed from Figure 1 that
\[
\begin{align*}
[a_1(1)] &= 0, \\
[a_6(2)] &= 0, \\
[a_7(3)] &= 0, \\
[a_{10}(4)] &= 28, \\
[a_{12}(5)] &= 86, \\
[a_{14}(6)] &= 164, \\
[a_{16}(7)] &= 264.
\end{align*}
\]

It implies that
\[
[a_{2n+1}(n)] = \left( \frac{(n-2)^3}{3} + 8(n-2)^2 + \frac{95}{3}(n-2) - 12 \right).
\]

(34)

In a similar fashion, we infer
\[
\begin{align*}
[a_{2n+1}(n)] &= \left( \frac{(n-3)^3}{3} + 10(n-3)^2 + \frac{149}{3}(n-4) - 16 \right), \\
[a_{2n+1}(n)] &= \left( \frac{(n-4)^3}{3} + 12(n-4)^2 + \frac{215}{3}(n-5) - 20 \right), \\
[a_{2n+1}(n)] &= \left( \frac{(n-5)^3}{3} + 14(n-5)^2 + \frac{293}{3}(n-6) - 24 \right), \\
\end{align*}
\]

\[
\begin{align*}
\ldots.
\end{align*}
\]

(35)

In terms of mathematical induction, we yield
\[
\begin{align*}
[a_{2n+1}(n)] &= \left( \frac{(n-(m/2))^3}{3} + \left( \frac{6(m/2)^2}{2} + 24(m/2) + 23 \right) \left( n - \frac{m}{2} \right) \right) \\
&\quad - 4 \left( \frac{m}{2} \right) - 4, \\
[a_{2n+1}(n)] &= \left( m + 4 \right) \left( \frac{m}{2} - n \right)^2 - \left( \frac{m}{2} - n \right)^3 \\
&\quad - 2m \left( \frac{m}{2} - n \right) \left( \frac{m^2}{2} + 4m + \frac{23}{3} \right) - 4, \\
[a_{2n+1}(n)] &= \left( \frac{m^3}{24} - \frac{m^2 n}{4} - \frac{m^2}{2} + \frac{mn^2}{2} - \frac{143m}{24} + \frac{n^3}{3} \\
&\quad - \frac{35m}{6} + \frac{23n}{3} - 4. \right.
\end{align*}
\]

(36)
Theorem 3. For the benzenoid hourglass system $X_{m}$, we have

(i) $W_{3}(X_{m}) = (3n^2 + 9n - 6) + (6n^2 + 12n - 12)2^{n}$
+ $\sum_{m=1}^{m \equiv 1 \mod (2),1 < m \leq 2n} \left( 19m^4/24 - 3m^2n - 5m^2 + 3mn^2 + 12mn + 221m/24 - 17 \right)x^m$

+ $\sum_{m=0}^{m \equiv 0 \mod (2),2 < m \leq 2n} \left( 19m^4/24 - 3m^2n - 5m^2 + 3mn^2 + 12mn + 59m/6 - 20 \right)x^m$

+ $\sum_{m=0}^{m \equiv 0 \mod (2),3 \leq m \leq 2n-2} \left( m^4/24 - m^2n/4 - m^2/2 - 143m/24 + n^3/3 + 4n^2 + 101n/12 - 5 \right)x^{2n-m}$

+ $\sum_{m=1}^{m \equiv 1 \mod (2),3 \leq m \leq 2n-2} \left( (m^4/2) - \frac{(m/2) - n}{3} - 2m - \frac{m^2}{2} - \frac{221m}{24} - 17 \right)x^{2n-m}$

+ $\sum_{m=0}^{m \equiv 0 \mod (2),2n-1 < m} \left( \frac{133m}{6} + \frac{11(n-1)^2}{2} + \frac{(n-1)^3}{3} - \frac{127}{6} \right)x^{2n+1} + \frac{1}{4n-1} \left( n^2 + 2 \right)x^{4n-1}.$

(ii) $W_{4}(X_{m}) = (3n^2 + 9n - 6)(1^4 + 1^{2^{3}}) + (6n^2 + 12n - 12)(2^4 + 2^{2^{3}}) + \sum_{m=1}^{m \equiv 1 \mod (2),1 < m \leq 2n} \left( 19m^4/24 - 3m^2n - 5m^2 + 3mn^2 + 12mn + 59m/6 - 20 \right)x^m$

+ $\sum_{m=0}^{m \equiv 0 \mod (2),2 < m \leq 2n} \left( 19m^4/24 - 3m^2n - 5m^2 + 3mn^2 + 12mn + 59m/6 - 20 \right)x^m$

+ $\sum_{m=0}^{m \equiv 0 \mod (2),3 \leq m \leq 2n-2} \left( m^4/24 - m^2n/4 - m^2/2 - 143m/24 + n^3/3 + 4n^2 + 101n/12 - 5 \right)x^{2n-m}$

+ $\sum_{m=1}^{m \equiv 1 \mod (2),3 \leq m \leq 2n-2} \left( (m^4/2) - \frac{(m/2) - n}{3} - 2m - \frac{m^2}{2} - \frac{221m}{24} - 17 \right)x^{2n-m}$

+ $\sum_{m=0}^{m \equiv 0 \mod (2),2n-1 < m} \left( \frac{133m}{6} + \frac{11(n-1)^2}{2} + \frac{(n-1)^3}{3} - \frac{127}{6} \right)x^{2n+1} + \frac{1}{4n-1} \left( n^2 + 2 \right)x^{4n-1}.$
$$
\sum_{m=0 \mod(2), 2 < m \leq 2n} ((19m^3/24) - 3m^2n - 5m^2 + 3mn^2 + 12mn + (59m/6 - 20)(m^4 + mn^3)) + \\
\sum_{m=0 \mod(2), 2 < m \leq 2n-2} ((m + 4)((m/2) - n)^3 - ((m/2) - n)^3/3 - 2m - (m/2) - n)((m/2) + 4m + (23/3) - 4)((2n + mn^3 + (2n + m)^{3/2} + (m/mn^2/4) - m^2 + (mn^2/2) - (143m/24) + (mn/3) + 4n^2 + (101n/12) - 5)((2n + m)^3 + (2n + m)^{3/2} + (133m/6) + (11(n - 1)^2/2 + ((n - 1)^3/3)) - \\
(127/6)((2n + 1)^3 + (2n + 1)^{3/2} + (n^2 + 2)((4n - 1)^3 + (4n - 1)^{3/2}).
$$

(iii) \( H_r(X_n) = (3n^3 + 9n - 6)(1/(1 + t)) + \\
(6n^3 + 12n - 12)(1/(2 + t)) + \\
\sum_{m=1 \mod(2), 1 < m \leq 2n} ((19m^3/24) - 3m^2n - 5m^2 + 3mn^2 + 12mn + (221m/24) - 17)(1/m + t) + \\
\sum_{m=0 \mod(2), 2 < m \leq 2n} ((19m^3/24) - 3m^2n - 5m^2 + 3mn^2 + 12mn + (59m/6 - 20)(1/m + t) + \\
\sum_{m=0 \mod(2), 2 < m \leq 2n-2} ((m + 4)((m/2) - n)^3 - ((m/2) - n)^3/3 - 2m - (m/2) - n)((m/2) - n)((m^2/2)4m + (23/3) - 1/2n + m + t) + \\
\sum_{m=1 \mod(2), 1 < m \leq 2n} ((m^3/24) - (m^2n/4) - m^3 + (m/2)^2 - (143m/24) + (n^3/3) + 4m^2 + (101n/12) - 5)((2n + m) + (133m/6) + (11(n - 1)^2/2) + \\
((n - 1)^3/3) - (127/6))((2n + 1)^3 + (2n + 1)^{3/2} + (n^2 + 2)((4n - 1)^3 + (4n - 1)^{3/2}).
$$

From the above theorem, we get the following results immediately.

**Corollary 1.** For the benzenoid hourglass system \( X_n \), we have

\[
W(X_n) = \frac{52n^5}{15} + \frac{80n^4}{15} + 34n^3 - \frac{116n^2}{3} - \frac{37n}{15} + 4. 
\]  

(42)

**Corollary 2.** For the benzenoid hourglass system \( X_n \), we have

\[
WW(X_n) = \frac{4n^5}{3} + 36n^4 + \frac{217n^3}{3} + 2n^2 + \frac{31n}{3} - 116
\]

\[
+ \sum_{m=1 \mod(2), 1 < m \leq 2n} m(m+1)\left(\frac{19m^3}{24} - 3m^2n - 5m^2 + 3mn^2 + 12mn + \frac{221m}{24} - 17\right)
\]

\[
+ \sum_{m=0 \mod(2), 2 < m \leq 2n} m(m+1)\left(\frac{19m^3}{24} - 3m^2n - 5m^2 + 3mn^2 + 12mn + \frac{59m}{6} - 20\right)
\]

\[
+ \sum_{m=0 \mod(2), 2 < m \leq 2n-2} \left(2n + m + (2n + m)^3\right)\left(m + 4\right)\left(\frac{m}{2} - n\right)^2 - \frac{((m/2) - n)^3}{3} - 2m - \frac{m - n}{3} - \frac{m^2 + 4m + 23}{3} - 4
\]

\[
+ \sum_{m=1 \mod(2), 1 < m \leq 2n-2} \left(2n + m + (2n + m)^3\right)\left(\frac{m^3}{24} - \frac{m^2n}{4} - m^3 + \frac{m^2}{2} - \frac{143m}{24} + \frac{n^3}{3} + 4n^2 + \frac{101n}{12} - 5\right).
\]

(43)

**Corollary 3.** The Harary index of benzenoid hourglass graph \( X_n \) is as follows:
\[
h(X_n) = \frac{296n^4 + 910n^3 - 161n^2 - 667n + 180}{6(8n^2 + 2n - 1)}
\]
\[
+ \sum_{m \equiv 1 \mod (2), 1 < m \leq 2n} \frac{1}{m} \left( \frac{19m^3}{24} - 3m^2 n - 5m^2 + 3mn^2 + 12mn + \frac{221m}{24} - 17 \right)
\]
\[
+ \sum_{m \equiv 0 \mod (2), 2 \leq m \leq 2n} \frac{1}{m} \left( \frac{19m^3}{24} - 3m^2 n - 5m^2 + 3mn^2 + 12mn + \frac{59m}{6} - 20 \right)
\]
\[
+ \sum_{m \equiv 1 \mod (2), 2 \leq m \leq 2n-2} \frac{1}{2n+m} \left( m + 4 \left( \frac{m-n}{2} \right)^3 - \frac{2}{3} \left( m-n \right) \left( \frac{m^2}{2} + 4m + \frac{23}{3} \right) - 4 \right)
\]
\[
+ \sum_{m \equiv 1 \mod (2), 3 \leq m \leq 2n-2} \frac{1}{2n+m} \left( m^3 - \frac{m^3}{4} - m^2 + \frac{mn^2}{2} - \frac{143m}{24} + \frac{n^3}{3} + 4n^2 + \frac{101n}{12} - 5 \right).
\]

4.2. Benzenoid Rhombus System. Consider a benzenoid system in which hexagons are arranged to form a rhombic shape, say, \( R_n \), where \( n \) represents number of hexagons along each boundary of the rhombic as given in Figure 2.

**Lemma 1.** The benzenoid rhombus system has \( 2n^2 + 4n \) vertices and \( 3n^2 + 4n - 1 \) edges.

**Theorem 4.** For the benzenoid rhombus system \( R_n \), we have

\[
H(R_n; x) = 2n^2 + 4n + (3n^2 + 4n - 1)x + (6n^2 + 4n - 4)x^2
\]
\[
+ \sum_{m \equiv 1 \mod (2), 1 < m \leq 2n} \left( 3mn^2 - 2m^2 n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{41m}{24} - 1 \right)x^m
\]
\[
+ \sum_{m \equiv 0 \mod (2), 2 \leq m \leq 2n} \left( 3mn^2 - 2m^2 n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{11m}{6} - 2 \right)x^m
\]
\[
+ \sum_{m \equiv 1 \mod (2), 1 \leq m \leq 2n-3} \left( \frac{(-m+2n-2)^3}{24} + \frac{(-m+2n-2)^2}{2} + \frac{23(-m+2n-2)^2}{24} - \frac{1}{2} \right)x^{2n+m+2}
\]
\[
+ \sum_{m \equiv 0 \mod (2), 2 \leq m \leq 2n-2} \left( \frac{(-m+2n)^3}{24} + \frac{(-m+2n)^2}{2} + \frac{5(-m+2n)^2}{6} \right)x^{2n+m}.
\]

**Proof.** To prove this theorem, we need to compute \( |a_m(n)| \)

where \( p = 1, 2, 3, \ldots, 2n+1 \). It is easy to verify that

\[
|a_0(n)| = |V| = 2n^2 + 4n,
\]
\[
|a_1(n)| = |E| = 3n^2 + 4n - 1,
\]
\[
|a_2(n)| = 6n^2 + 4n - 4.
\]

The remaining proof is divided into two parts which are according to the parity of \( m \).

**Case 7.** \( m \equiv 1 \mod (2), 1 < m \leq 2n + 1 \).

It can be observed from Figure 2 that \( |a_3(n)| = 9n^2 - 6 \).

In a similar fashion, we have
interms of mathematical induction, we yield

\[ a_m(n) = 3m \left( n - \frac{m-3}{2} \right)^2 + \left( m^2 - 3m \right) \left( n - \frac{m-3}{2} \right) + \frac{1}{24} m^3 - \frac{1}{2} m^2 - \frac{13}{24} m - 1, \]

\[ a_m(n) = 3mn^2 - 2m^2 n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{41m}{24} - 1. \]  

(52)

Case 8. \( m \equiv 0 \mod(2), 2 < m \leq 2n. \)

It can be observed from Figure 2 that

\[ a_4(1) = 0, \]
\[ a_4(2) = 24, \]
\[ a_4(3) = 76, \]
\[ a_4(4) = 152, \]
\[ a_4(5) = 252. \]  

(53)

Now, one can conclude that

\[ a_4(n) = 12(n-1)^2 + 16(n-1) - 4. \]  

(54)

By means of the same trick, we obtain

\[ a_6(1) = 0, \]
\[ a_6(2) = 0, \]
\[ a_6(3) = 54, \]
\[ a_6(4) = 144, \]
\[ a_6(5) = 270, \]
\[ a_6(6) = 432, \]  

(55)

which reveals that

\[ a_6(n) = 18(n-2)^2 + 36 \ast (n-2). \]  

(56)

In light of the similar approach, we get

\[ a_{10}(n) = 24(n-3)^2 + 64(n-3) + 10, \]
\[ a_{10}(n) = 30(n-4)^2 + 100(n-4) + 28, \]
\[ a_{12}(n) = 36(n-5)^2 + 144(n-5) + 56, \]  

\[ \ldots. \]  

(57)

Hence, by mathematical induction, we have

\[ a_m(n) = 3m \left( n - \frac{m+1}{2} \right)^2 + m^2 \left( n - \frac{m+1}{2} \right) + \frac{1}{24} m^3 - \frac{7}{6} m - 2, \]

\[ a_m(n) = 3mn^2 - 2m^2 n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{11m}{6} - 2. \]  

(58)
Now for \( m = 2n + 2 \) to \( m = 4n - 1 \), we will generalize in this way. By observing Table 1, values in italics show the distances from \( 2n + 2 \) to \( 4n - 1 \), but the values in the table are in descending order, so first we generalized this in ascending order and then reverse its order as required, let \( p_i \) be the values in ascending order as follows (from Table 1).

\[
\begin{align*}
p_1 &= 1, \\
p_2 &= 4, \\
p_3 &= 8, \\
p_4 &= 14, \\
p_5 &= 22, \\
p_6 &= 32, \\
p_7 &= 45, \\
p_8 &= 60, \\
p_9 &= 79, \\
p_{10} &= 100.
\end{align*}
\]

**Case 9.** \( i \equiv 1 \text{mod}(2) \).

Hence, one can conclude that

\[ p_1 = \frac{i^3}{24} + \frac{i^2}{2} + \frac{23i}{24} - \frac{1}{2} \]  

(60)\[ \text{For } m \equiv \text{mod}(2), 1 \leq m \leq 2n - 3. \]

So to reverse its order put \( i = (-m + 2n - 2) \), we get

\[
|a_{m}(n)| = \frac{(-m + 2n - 2)^3}{24} + \frac{(-m + 2n - 2)^2}{2} + \frac{23(-m + 2n - 2)}{24} - \frac{1}{2} \]  

(61)

**Case 10.** \( i \equiv 0 \text{mod}(2) \).

Hence, one can conclude that

\[ p_1 = \frac{i^3}{24} + \frac{i^2}{2} + \frac{5i}{6} \]  

(62)

For \( m \equiv \text{mod}(2), 2 \leq m \leq 2n - 2 \).

So to reverse its order put \( i = (-m + 2n) \), we get

\[
|a_{m}(n)| = \frac{(-m + 2n)^3}{24} + \frac{(-m + 2n)^2}{2} + \frac{5(-m + 2n)}{6} \]  

(63)

By what has been mentioned above, we get our desired result.

**Theorem 5.** For the benzenoid rhombus system \( R_n \), the Hary polynomial is as follows:

\[
h(R_n; x) = (3n^2 + 4n - 1)x + (3n^2 + 2n - 2)x^2
\]

\[
+ \sum_{m = 1 \text{mod}(2), 1 < m \leq 2n + 1} \frac{1}{m} \left( \frac{3mn^2 - 2m^2n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{41m}{24}}{2} - 1 \right) x^m
\]

\[
+ \sum_{m = 0 \text{mod}(2), 2 < m \leq 2n} \frac{1}{m} \left( \frac{3mn^2 - 2m^2n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{11m}{6} - 2}{2} \right) x^m
\]

\[
+ \sum_{m = 1 \text{mod}(2), 1 \leq m \leq 2n - 3} \frac{1}{2n + m + 2} \left( \frac{(-m + 2n - 2)^3}{24} + \frac{(-m + 2n - 2)^2}{2} + \frac{23(-m + 2n - 2)}{24} - \frac{1}{2} \right) x^{2n+m+2}
\]

\[
+ \sum_{m = 0 \text{mod}(2), 2 \leq m \leq 2n - 2} \frac{1}{2n + m} \left( \frac{(-m + 2n)^3}{24} + \frac{(-m + 2n)^2}{2} + \frac{5(-m + 2n)}{6} \right) x^{2n+m}.
\]

**Proof.** From the information about the number of pairs of vertices at different distances given in Theorem 4, one can easily get this result. \( \square \)

**Theorem 6.** For the benzenoid rhombus system \( R_n \), we have

\begin{enumerate}[label=(i)]
\item \[ W_{\lambda}(R_n) = (3n^2 + 4n - 1) + (6n^2 + 4n - 4)2^k \]
\item \[ \sum_{m = 1 \text{mod}(2), 1 < m \leq 2n + 1} \left( \frac{3mn^2 - 2m^2n + (7m^3)/24 + 6mn - 2m^2 + (41m/24) - 1}{m} \right) + \\
\sum_{m = 0 \text{mod}(2), 2 < m \leq 2n} \left( \frac{3mn^2 - 2m^2n + (7m^3)/24 + 6mn - 2m^2 + (41m/24) - 1}{m} \right) + \]
\item \[ \sum_{m = 0 \text{mod}(2), 2 < m \leq 2n} \left( \frac{3mn^2 - 2m^2n + (7m^3)/24 + 6mn - 2m^2 + (41m/24) - 1}{m} \right) + \]
\end{enumerate}
Table 1: Number of pair of vertices at different distances.

| Distance (m) | n   |
|-------------|-----|
| 1           | 174 |
| 2           | 318 |
| 3           | 435 |
| 4           | 524 |
| 5           | 589 |
| 6           | 630 |
| 7           | 650 |
| 8           | 650 |
| 9           | 632 |
| 10          | 598 |
| 11          | 549 |
| 12          | 488 |
| 13          | 415 |
| 14          | 334 |
| 15          | 244 |
| 16          | 154 |
| 17          | 126 |
| 18          | 100 |
| 19          | 79  |
| 20          | 74  |
| 21          | 74  |
| 22          | 88  |
| 23          | 88  |
| 24          | 88  |
| 25          | 88  |
| 26          | 88  |
| 27          | 1   |

\[ 2m^2 + (11m/6) - 2) (m^4 + n^{23}) + \sum_{n \equiv 1 \text{mod}(2), 1 \leq m \leq 2n} (3m^2 - 2m^2 n + 7m^3/24 + 6mn - 2m^2 - 41m/24 - 1) \]

\[ + \sum_{n \equiv 0 \text{mod}(2), 2 \leq m \leq 2n} (3m^2 - 2m^2 n + 7m^3/24 + 6mn - 2m^2 + 11m/6 - 2) \]

\[ + \sum_{n \equiv 1 \text{mod}(2), 1 \leq m \leq 2n} (2n + m + 2 + (2n + m + 2)^2) \times \left( \frac{(-m + 2n - 2)\text{mod}(2)}{24} + \frac{(-m + 2n - 2)^2}{2} + \frac{23(-m + 2n - 2)\text{mod}(2)}{24} - 1 \right) \]

\[ + \sum_{n \equiv 0 \text{mod}(2), 2 \leq m \leq 2n} (2n + m + (2n + m)^2) \times \left( \frac{(-m + 2n)\text{mod}(2)}{24} + \frac{(-m + 2n)^2}{2} + 5(-m + 2n)\text{mod}(2)/6 - 1 \right) \]

From the above results, we get the following results immediately.

**Corollary 4.** For the benzenoid rhombus system \( R_m \), we have

\[ W(R_n) = \frac{34n^2}{15} + \frac{34n^4}{3} + \frac{40n^6}{3} + \frac{2n^8}{3} - \frac{3n}{5} \tag{65} \]

**Corollary 5.** For the benzenoid rhombus system \( R_m \), we have

\[ WW(R_n) = 42n^2 + 32n - 26 \]

\[ + \sum_{n \equiv 1 \text{mod}(2), 1 \leq m \leq 2n+1} m(m + 1) \left( 3m^2 - 2m^2 n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{41m}{24} - 1 \right) \]

\[ + \sum_{n \equiv 0 \text{mod}(2), 2 \leq m \leq 2n} m(m + 1) \left( 3m^2 - 2m^2 n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{11m}{6} - 2 \right) \]

\[ + \sum_{n \equiv 1 \text{mod}(2), 1 \leq m \leq 2n-3} (2n + m + 2 + (2n + m + 2)^2) \times \left( \frac{(-m + 2n - 2)\text{mod}(2)}{24} + \frac{(-m + 2n - 2)^2}{2} + \frac{23(-m + 2n - 2)\text{mod}(2)}{24} - 1 \right) \]

\[ + \sum_{n \equiv 0 \text{mod}(2), 2 \leq m \leq 2n-2} (2n + m + (2n + m)^2) \times \left( \frac{(-m + 2n)\text{mod}(2)}{24} + \frac{(-m + 2n)^2}{2} + 5(-m + 2n)\text{mod}(2)/6 - 1 \right) \]
Corollary 6. The Harary index of benzenoid rhombus graph $R_n$ is as follows:

$$h(R_n) = 6n^2 + 6n - 3 + \sum_{m \equiv 1 \mod 2, 1 < m \leq 2n-1} \frac{1}{m} \left( 3mn^2 - 2m^2n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{41m}{24} - 1 \right)$$

$$+ \sum_{m \equiv 0 \mod 3, 2 < m \leq 2n} \frac{1}{m} \left( 3mn^2 - 2m^2n + \frac{7m^3}{24} + 6mn - 2m^2 + \frac{11m}{6} - 2 \right)$$

$$+ \sum_{m \equiv 1 \mod 2, 1 \leq m \leq 2n-3} \frac{1}{2n + m + 2} \left( \frac{(-m + 2n - 2)^3}{24} + \frac{(-m + 2n - 2)^2}{2} + \frac{23(-m + 2n - 2)}{24} - \frac{1}{2} \right)$$

$$+ \sum_{m \equiv 0 \mod 2, 3 \leq m \leq 2n-2} \frac{1}{2n + m} \left( \frac{(-m + 2n)^3}{24} + \frac{(-m + 2n)^2}{2} + \frac{5(-m + 2n)}{6} \right) \tag{67}$$

5. Conclusions

Wiener demonstrated that the Wiener index is firmly connected to the boiling point of alkane. Later work on quantitative structure-activity connections demonstrated that it is additionally corresponded to different amounts including the parameters of its basic point the thickness, surface strain, and consistency of its fluid stage and the van der Waals surface territory of the molecules. Wiener index is a valuable topological index in the structure-property relationship since it is the measurement of compactness of particle regarding its basic characteristics, for example, spreading and cyclicity. Utilizations of benzene follow a long history. In the nineteenth and midtwentieth centuries, benzene was utilized as an aftershave lotion due to its wonderful smell. Before the 1920s, benzene was as often as possible utilized as a modern dissolvable, particularly to degrease metal. As its lethality wound up self-evident, benzene was displaced by different solvents, particularly toluene (methylbenzene), which has comparable physical properties yet is not as cancer-causing. In 1903, Ludwig Roselius promoted the utilization of benzene to decaffeinate espresso. This disclosure prompted the creation of Sanka. This procedure was later ended. Benzene was generally utilized as a noteworthy part in numerous shopper items, for example, Liquid Wrench, a few paint strippers, elastic concretes, spot removers, and different items. Produce of ample, Liquid Wrench, a few paint strippers, elastic

Data Availability

All the data are included within this paper.

Conflicts of Interest

The authors of this paper declare that they have no conflicts of interest.

Authors’ Contributions

All authors have equal contribution.

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