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HOSOYA POLYNOMIAL AND WIENER INDEX OF CONCATENATED OCTACHAINS

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Abstract. Wiener index of a connected graph $G = (V, E)$ is defined as $W(G) = \sum_{\{u,v\}\subset V(G)} d(u, v)$ and Hosoya polynomial is defined as $H(G, x) = \sum_{\{u,v\}\subset V(G)} x^{d(u,v)}$. In this paper, Wiener index and Hosoya polynomials of several types of graphs consisting of concatenated octagon rings which are used in chemistry, pharmacology and materials science are obtained.

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1. Introduction

Nowadays, graph theory has numerous applications in such diverse fields as electronics, sociology, nuclear physics, computer science, ethnology, engineering, geography, linguistics, biology, transportation, and particularly in chemistry and all sciences using molecular studies. Numerous books, [4, 13], and review articles, [3, 5, 6, 7, 8, 9, 11, 12, 14], have been written on the applications of graphs in chemistry. Especially, the mathematical study of nano-dimensional materials in physics, chemistry, textile, civil engineering, pharmacology, climatology, etc. is becoming one of the most interesting interdisciplinary research areas, see e.g. [1, 2, 15, 16].

In 1947, Harold Wiener published a paper, [14], in which Wiener index or Wiener number was introduced for the first time and he used his index for the calculation of the boiling points of alkanes. Wiener's formula for the boiling points bp is

$$bp = \alpha W + \beta P + \gamma$$

where α, β, γ are empirical constants and P, the polarity number, is the number of pairs of vertices with distance equal to three. He used Wiener index to predict boiling points, molar volumes, refractive indices, heats of isomerization and heats of vaporization of alkanes. Chemical applications of the Wiener index are outlined in the articles [3, 10].

Let G be a connected graph. The Wiener index of the graph $G = (V, E)$ is defined as

$$W(G) = \sum_{\{u,v\}\subset V(G)} d(u, v)$$

where $d(u,v)$ is the minimum of the lengths of all $u-v$ paths in G, i.e., the shortest path between the vertices u and v. The Hosoya polynomial (also called Wiener polynomial) of G is defined as

$$H(G,x)=\sum_{\{u,v\}\subset V(G)} x^{d(u,v)}.$$

It is clear that

$$H(G,x)=\sum_{k\geq 0} d(G,k)x^k,$$

where $d(G,k)$ is the number of pairs (u,v) of vertices of G such that $d(u,v)=k$. The Hosoya polynomial of a vertex v of G is defined as

$$H(v,G;x)=\sum_{k\geq 1} d(v,G,k)x^k,$$

in which $d(v,G,k)$ is the number of all vertices u belonging to $V(G)$, such that $d(u,v)=k$. The Wiener index of G can be obtained directly from the Hosoya polynomial of G as follows:

$$W(G)=\frac{d}{dx}(H(G,x))|_{x=1}.$$

In this paper, the Hosoya polynomial and Wiener index for several types of graphs consisting of concatenated octagon rings are obtained. The rest of the paper is organized as follows: In Section 2, three types of straight octagonal chains denoted by $G(n,S_1)$, $G(n,S_2)$ and $G(n,S_3)$ are defined and their Hosoya polynomials are calculated. Depending on the edge structure of these chains, the Wiener indexes are calculated. In Section 3, using two rows of $G(n,S_1)$ and $G(n,S_3)$, two more straight octagonal chains denoted by $G(n,S_4)$ and $G(n,S_5)$ are introduced and their Hosoya polynomials and Wiener indices are obtained.

2. Straight Octagonal Chains

A straight octagonal chain is a graph consisting of n octagonal rings where every two successive rings have a common edge, forming a chain denoted by $G(n,S_1)$ as shown in Fig. 2.1. The number of vertices in $G(n,S_1)$ is $6n+2$ and of edges is $7n+1$. The Hosoya polynomial of the graph $G(n,S_1)$ is obtained in the next theorem:

Theorem 2.1. *For $n\geq 2$, the Hosoya polynomial of the chain $G(n,S_1)$ is given by*

$$H(G(n,S_1))=(7n+1)x+(10n-2)x^2+(14n-6)x^3+(14n-10)x^4+\sum_{k=5}^{3n+1}(4(3n-k)+6)x^k.$$

Proof. We prove this theorem using mathematical induction on n for $n\geq 2$.

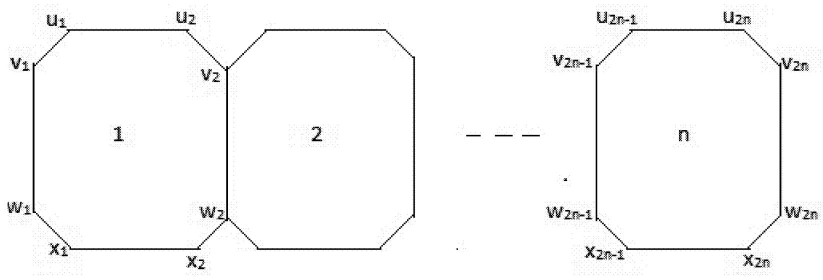

Figure 2.1

For $n = 2$, we have by direct calculation

$$H(G(2, S_1)) = 15x + 18x^2 + 22x^3 + 18x^4 + 10x^5 + 6x^6 + 2x^7.$$

Thus the theorem is true for $n = 2$.

Let us assume that the theorem is true for $n = r \geq 2$ and we prove that it is true for $n = r + 1$. It is clear from Fig. 2.1 that

$$H(G(r + 1, S_1)) = H(G(r, S_1)) + g(x),$$

where

$$g(x) = \sum_{i=1}^{6} H(a_i, G(r + 1, S_1)) - 5x - 4x^2 - 4x^3 - 2x^4.$$

Here $a_1 = u_{2r+1},\ a_2 = u_{2r+2},\ a_3 = v_{r+2},\ a_4 = w_{r+2},\ a_5 = x_{2r+2},\ a_6 = x_{2r+1}$. But by the symmetry property, we also have

$$H(u_{2r+1}, G(r + 1, S_1)) = H(x_{2r+1}, G(r + 1, S_1)).$$

Hence we can write

$$H(u_{2r+2}, G(r + 1, S_1)) = H(x_{2r+2}, G(r + 1, S_1))$$

and

$$H(v_{r+2}, G(r + 1, S_1)) = H(w_{r+2}, G(r + 1, S_1)).$$

So

$$\begin{aligned} g(x) &= 2(H(u_{2r+1}, G(r + 1, S_1)) + H(u_{2r+2}, G(r + 1, S_1)) + H(v_{r+2}, G(r + 1, S_1))) \\ &\quad -5x - 4x^2 - 4x^3 - 2x^4. \end{aligned}$$

Also

$$H(u_{2r+1}, G(r + 1, S_1)) = 2x + 3x^2 + 4x^3 + 3x^4 + 2\sum_{k=5}^{3r+1} x^k + x^{3r+2},$$

$$H(u_{2r+2}, G(r + 1, S_1)) = 2x + 2x^2 + 3x^3 + 3x^4 + 2\sum_{k=5}^{3r+2} x^k + x^{3r+3}$$

and

$$H(w_{r+1}, G(r + 1, S_1)) = 2\sum_{k=1}^{3r+3} x^k + x^{3r+4}.$$

Hence

$$g(x) = 7x + 10x^2 + 14x^3 + 14x^4 + 12\sum_{k=5}^{3r+1} x^k + 10x^{3r+2} + 6x^{3r+3} + 2x^{3r+4}.$$

Thus

$$\begin{aligned} H(G(r+1, S_1)) &= (7r+1)x + (10r-2)x^2 + (14r-6)x^3 + (14r-10)x^4 \\ &\quad + \textstyle\sum_{k=5}^{3r+1}(4(3r-k)+6)x^k + 7x + 10x^2 + 14x^3 + 14x^4 \\ &\quad + 12\textstyle\sum_{k=5}^{3r+1} x^k + 10x^{3r+2} + 6x^{3r+3} + 2x^{3r+4} \\ &= (7(r+1)+1)x + (10(r+1)-2)x^2 + (14(r+1)-6)x^3 \\ &\quad + (14(r+1)-10)x^4 + \textstyle\sum_{k=5}^{3(r+1)+1}(4(3(r+1)-k)+6)x^k. \end{aligned}$$

Hence the result is true for all $n \geq 2$. □

We know that $H(G(1, S_1)) = 8x + 8x^2 + 8x^3 + 4x^4$, so we can obtain $H(G(n, S_1))$ for all natural numbers n.

Theorem 2.2. *For $n \geq 2$, the Wiener index of $G(n, S_1)$ is given by*

$$W(G(n, S_1)) = 18n^3 + 27n^2 + 18n + 1.$$

Proof. Wiener index can be obtained by taking derivative of $H(G(n, S_1))$ with respect to x and then putting $x = 1$.

$$\begin{aligned} W(G(n, S_1)) &= \frac{d}{dx}(H(G(n, S_1)))_{x=1} \\ &= (7n+1) + 2(10n-2) + 3(14n-6) + 4(14n-10) \\ &\quad + \textstyle\sum_{k=5}^{3n+1} k(4(3n-k)+6) \\ &= 125n - 61 + (12n+6)\textstyle\sum_{k=5}^{3n+1} k - 4\textstyle\sum_{k=5}^{3n+1} k^2 \\ &= 18n^3 + 27n^2 + 18n + 1. \end{aligned}$$

Hence we find

$$W(G(n, S_1)) = 18n^3 + 27n^2 + 18n + 1,$$

for $n \geq 2$. As we can easily calculate $W(G(1, S_1)) = 64$, we can obtain $W(G(n, S_1))$ for all natural numbers n. □

Now we consider another chain graph which will be denoted by $G(n, S_2)$ consisting of n octagonal rings where every two successive rings have a common edge as shown in Fig. 2.2. The number of vertices and edges in $G(n, S_2)$ are $6n + 2$ and $7n + 1$, respectively.

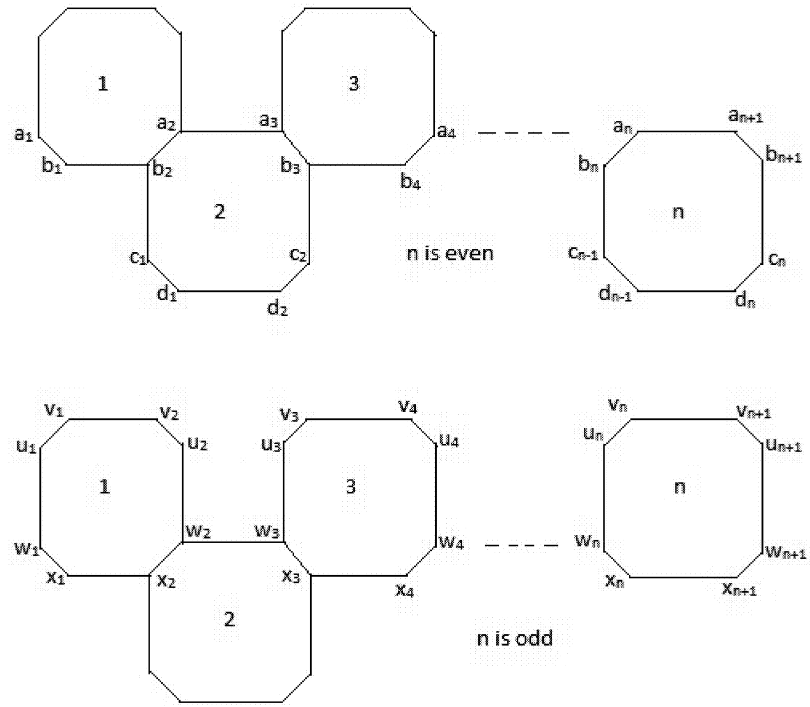

Figure 2.2

Theorem 2.3. *For $n \geq 6$, the Hosoya polynomial of $G(n, S_2)$ is given by*

$$\begin{aligned} H(G(n,S_2)) &= (7n+1)x + (10n-2)x^2 + (15n-8)x^3 + 18(n-1)x^4 \\ &+ (19n-29)x^5 + (20n-38)x^6 + (19n-46)x^7 + (18n-54)x^8 \\ &+ \sum_{k=9}^{2n}(18(n+1)-9k)x^k + 10x^{2n+1} + 4x^{2n+2} + x^{2n+3}. \end{aligned}$$

Proof. We prove this theorem by mathematical induction on n, for $n \geq 6$. By direct calculation, we have

$$\begin{aligned} H(G(6,S_2)) &= 43x + 58x^2 + 82x^3 + 90x^4 + 85x^5 + 82x^6 + 68x^7 + 54x^8 + 45x^9 + 36x^{10} \\ &+ 27x^{11} + 18x^{12} + 10x^{13} + 4x^{14} + x^{15} \end{aligned}$$

and

$$\begin{aligned} H(G(7,S_2)) &= 50x + 68x^2 + 97x^3 + 108x^4 + 104x^5 + 102x^6 + 87x^7 + 72x^8 + 63x^9 \\ &+ 54x^{10} + 45x^{11} + 36x^{12} + 27x^{13} + 18x^{14} + 10x^{15} + 4x^{16} + x^{17}. \end{aligned}$$

Thus the theorem is true for n = 6 and 7.

Let us next assume that the statement is true for $n = r \geq 6$ and prove that it is true for $n = r+1$. It is clear from Fig. 2.2 that

(1) $$H(G(r+1,S_2)) = H(G(r,S_2)) + g(x)$$

where

$$g(x)=\sum_{i=1}^{6}H(m_i,G(r+1,S_2))-5x-4x^2-4x^3-2x^4$$

with

$$m_1=a_{r+2},\ m_2=b_{r+2},\ m_3=c_{r+1},\ m_4=d_{r+1},\ m_5=d_r,\ m_6=c_r$$

for r is odd and

$$m_1=v_{r+1},m_2=v_{r+2},m_3=u_{r+1},m_4=u_{r+2},m_5=w_{r+2},m_6=x_{r+1}$$

for r is even.

Case 1. If r is odd, then

$$H(a_{r+2},G(r+1,S_2))=2x+3x^2+4x^3+4x^4+3\sum_{k=5}^{2r+1}x^k+2x^{2r+2}+x^{2r+3},$$

$$H(b_{r+2},G(r+1,S_2))=2x+2x^2+3\sum_{k=3}^{2r+2}x^k+2x^{2r+3}+x^{2r+4},$$

$$H(c_{r+1},G(r+1,S_2))=2x+2x^2+2x^3+2x^4+2x^5+3\sum_{k=6}^{2r+3}x^k+2x^{2r+4}+x^{2r+5},$$

$$H(d_{r+1},G(r+1,S_2))=2x+2x^2+2x^3+2x^4+3x^5+4x^6+4x^7+3\sum_{k=8}^{2r+2}x^k+2x^{2r+3}+x^{2r+4},$$

$$H(d_r,G(r+1,S_2))=2x+2x^2+3x^3+4x^4+4x^5+4x^6+3\sum_{k=7}^{2r+1}x^k+2x^{2r+2}+x^{2r+3},$$

and

$$H(c_r,G(r+1,S_2))=2x+3x^2+5x^3+5x^4+4x^5+3\sum_{k=6}^{2r}x^k+2x^{2r+1}+x^{2r+2}.$$

Thus

$$\begin{aligned}g(x)\ &=\ 7x+10x^2+15x^3+18x^4+19x^5+20x^6+19x^7+18x^8\\&\quad+18\textstyle\sum_{k=9}^{2r}x^k+17x^{2r+1}+14x^{2r+2}+10x^{2r+3}+4x^{2r+4}+x^{2r+5}.\end{aligned}$$

From (1), we have

$$\begin{aligned}H(G(r+1,S_2))\ &=\ (7(r+1)+1)x++(10(r+1)-2)x^2+(15(r+1)-8)x^3\\&\quad+18((r+1)-1)x^4+(19(r+1)-29)x^5+(20(r+1)-38)x^6\\&\quad+(19(r+1)-46)x^7+(18(r+1)-54)x^8\\&\quad+\textstyle\sum_{k=9}^{2(r+1)}(18((r+1)+1)-9k)x^4\\&\quad+10x^{2(r+1)+1}+4x^{2(r+1)+2}+x^{2(r+1)+3}.\end{aligned}$$

Hence the result.

Case II. If r is even, then we have

$$H(v_{r+1},G(r+1,S_2))=2x+2x^2+3x^3+4x^4+4x^5+4x^6+3\sum_{k=7}^{2r+1}x^k+2x^{2r+2}+x^{2r+3},$$

$$H(v_{r+2}, G(r+1, S_2)) = 2x+2x^2+2x^3+2x^4+3x^5+4x^6+4x^7+3\sum_{k=8}^{2r+2} x^k+2x^{2r+3}+x^{2r+4},$$

$$H(u_{r+1}, G(r+1, S_2)) = 2x+3x^2+5x^3+5x^4+4x^5+3\sum_{k=6}^{2r} x^k+2x^{2r+1}+x^{2r+2},$$

$$H(u_{r+2}, G(r+1, S_2)) = 2x+2x^2+2x^3+2x^4+2x^5+3\sum_{k=6}^{2r+3} x^k+2x^{2r+4}+x^{2r+5},$$

$$H(w_{r+2}, G(r+1, S_2)) = 2x + 2x^2 + 3\sum_{k=3}^{2r+2} x^k + 2x^{2r+3} + x^{2r+4},$$

and

$$H(x_{r+2}, G(r+1, S_2)) = 2x + 3x^2 + 4x^3 + 4x^4 + 3\sum_{k=5}^{2r+1} x^k + 2x^{2r+2} + x^{2r+3}.$$

Thus

$$\begin{aligned} g(x) &= 7x + 10x^2 + 15x^3 + 18x^4 + 19x^5 + 20x^6 + 19x^7 + 18x^8 \\ &\quad +18\textstyle\sum_{k=9}^{2r} x^k + 17x^{2r+1} + 14x^{2r+2} + 10x^{2r+3} + 4x^{2r+4} + x^{2r+5}. \end{aligned}$$

From (1), we obtain

$$\begin{aligned} H(G(r+1, S_2)) &= (7(r+1)+1)x + (10(r+1)-2)x^2 + (15(r+1)-8)x^3 \\ &\quad +18((r+1)-1)x^4 + (19(r+1)-29)x^5 + (20(r+1)-38)x^6 \\ &\quad +(19(r+1)-46)x^7 + (18(r+1)-54)x^8 \\ &\quad +\textstyle\sum_{k=9}^{2(r+1)}(18((r+1)+1)-9k)x^k \\ &\quad +10x^{2(r+1)+1} + 4x^{2(r+1)+2} + x^{2(r+1)+3}. \end{aligned}$$

Hence the result. □

Note that the Hosoya polynomials of $G(n, S_2)$, for $1 \le n \le 5$, are given below:

$$H(G(1, S_2)) = H(G(1, S_1)),$$

$$H(G(2, S_2)) = 15x + 18x^2 + 22x^3 + 18x^4 + 10x^5 + 6x^6 + 2x^7,$$

$$H(G(3, S_2)) = 22x + 28x^2 + 37x^3 + 36x^4 + 28x^5 + 22x^6 + 12x^7 + 4x^8 + x^9,$$

$$H(G(4, S_2)) = 29x+38x^2+52x^3+54x^4+47x^5+42x^6+30x^7+18x^8+10x^9+4x^{10}+x^{11}$$

and

$$\begin{aligned} H(G(5, S_2)) &= 36x + 48x^2 + 67x^3 + 72x^4 + 66x^5 + 62x^6 + 49x^7 + 36x^8 + 27x^9 \\ &\quad +18x^{10} + 10x^{11} + 4x^{12} + x^{13}. \end{aligned}$$

Thus we can obtain $H(G(n, S_2))$ for all natural numbers n.

Theorem 2.4. *For $n \ge 6$, the Wiener index of $G(n, S_2)$ is given by*

$$W(G(n, S_2)) = 12n^3 + 36n^2 + 33n - 17.$$

Proof. Wiener index can be obtained by taking derivative of $H(G(n,S_2))$ with respect to x and then putting $x=1$.

$$\begin{aligned} W(G(n,S_2)) &= \tfrac{d}{dx}(H(G(n,S_2)))_{x=1} \\ &= (7n+1)+2(10n-2)+3(15n-8)+72(n-1) \\ &\quad +5(19n-29)+6(20n-38)+7(19n-46)+8(18n-54) \\ &\quad +10(2n+1)+4(2n+2)+(2n+3)+(18n+1)\textstyle\sum_{k=9}^{2n}k \\ &\quad -\textstyle\sum_{k=9}^{2n}k^2 \\ &= 12n^3+36n^2+33n-17 \end{aligned}$$

for $n \geq 6$.

The above formula is valid for all n except $n=3$ and in that case we have $W(G(3,S_2)) = 734$. Hence we can obtain $W(G(n,S_2))$ for all natural numbers n. □

Now we consider another structure which will be denoted by $G(n,S_3)$ consisting of $n/2$ octagons and $n/2$ squares where between two consecutive octagons there is a square, as shown in Fig. 2.3. The number of vertices and edges in $G(n,S_3)$ are $8n+2$ and $10n+1$, respectively.

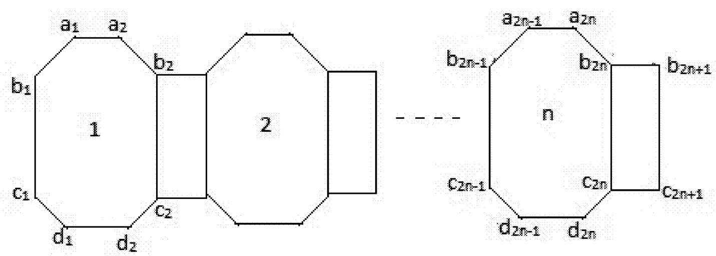

Figure 2.3

Theorem 2.5. *For $n \geq 2$, the Hosoya polynomial of $G(n,S_3)$ is given by*

$$\begin{aligned} H(G(n,S_3)) &= (10n+1)x+(14n-2)x^2+(18n-6)x^3+(18n-10)x^4 \\ &\quad +\textstyle\sum_{k=5}^{4n+1}(16n-(4k-6))x^k. \end{aligned}$$

Proof. We use mathematical induction on n for $n \geq 2$. First for $n=2$, we find by direct calculation that $H(G(2,S_3)) = 21x+26x^2+30x^3+26x^4+18x^5+14x^6+10x^7+6x^8+2x^9$. Thus, (1) is true for $n=2$. We assume that (1) is true for $n=r \geq 2$ and prove that it is true for $n=r+1$. It is clear from Fig. 2.4 that

$$H(G(r+1,S_3)) = H(G(r,S_3)) + g(x),$$

where

$$g(x) = \sum_{i=1}^{8} H(m_i, G(r+1,S_3)) - (8x+8x^2+8x^3+4x^4).$$

Here $m_1 = d_{2r+1}$, $m_2 = d_{2r+2}$, $m_3 = c_{2r+2}$, $m_4 = c_{2r+3}$, $m_5 = b_{2n+3}$, $m_6 = b_{2n+2}$, $m_7 = a_{2n+2}$, $m_8 = a_{2n+1}$ and

$$\begin{aligned} H(m_1, G(r+1, S_3)) &= 2x + 3x^2 + 5x^3 + 4x^4 + 2\sum_{k=5}^{4r+1} x^k + x^{4r+2} \\ &= H(w_8, G(r+1, S_3)), \end{aligned}$$

$$\begin{aligned} H(m_2, G(r+1, S_3)) &= 2x + 3x^2 + 4x^3 + 3x^4 + 2\sum_{k=5}^{4r+2} x^k + x^{4r+3} \\ &= H(w_7, G(r+1, S_3)), \end{aligned}$$

$$\begin{aligned} H(m_3, G(r+1, S_3)) &= 3\sum_{k=1}^{2} x^k + \sum_{k=3}^{4r+3} x^k + x^{4r+4} \\ &= H(w_6, G(r+1, S_3)), \end{aligned}$$

$$\begin{aligned} H(m_4, G(r+1, S_3)) &= 2\sum_{k=1}^{4r+4} x^k + x^{4r+5} \\ &= H(w_5, G(r+1, S_3)). \end{aligned}$$

Thus,

$$\begin{aligned} H(G(r+1, S_3)) &= (10r+1)x + (14r-2)x^2 + (18r-6)x^3 + (18r-10)x^4 \\ &\quad + \sum_{k=5}^{4r+1}(16r-(4k-6))x^k + 10x + 14x^2 + 18x^3 + 18x^4 \\ &\quad + 16\sum_{k=5}^{4r+1} x^k + 14x^{4r+2} + 10x^{4r+3} + 6x^{4r+4} + 2x^{4r+5} \\ &= (10(r+1)+1)x + (14(r+1)-2)x^2 + (18(r+1)-6)x^3 \\ &\quad + (18(r+1)-10)x^4 + \sum_{k=5}^{4(r+1)+1}(16(r+1)-(4k-6))x^k. \end{aligned}$$

Hence the result is true for all n, $n \geq 2$, which completes the proof. □

Note that the Hosoya polynomial of $G(1, S_3)$ is

$$H(G(1, S_3)) = 11x + 12x^2 + 12x^3 + 8x^4 + 2x^5.$$

Thus we can obtain $H(G(n, S_3))$ for all natural numbers n.

Theorem 2.6. *For $n \geq 2$, the Wiener index of $G(1, S_3)$ is given by*

$$W(G(n, S_3)) = \frac{1}{3}(128n^3 + 144n^2 + 64n + 3).$$

Proof. Wiener index can be obtained by taking derivative of $H(G(n, S_3))$ with respect to x and then substituting $x = 1$. The $W(G(1, S_3)) = 113$, hence we can obtain Wiener index for all natural numbers n. □

3. Octagonal chains in two rows

In this section, we consider another type of chain graphs which will be denoted by $G(n, S_4)$ and will be formed by means of two rows of $G(n, S_3)$ as shown in Fig. 3.1. It contains $16n + 4$ vertices and $22n + 2$ edges.

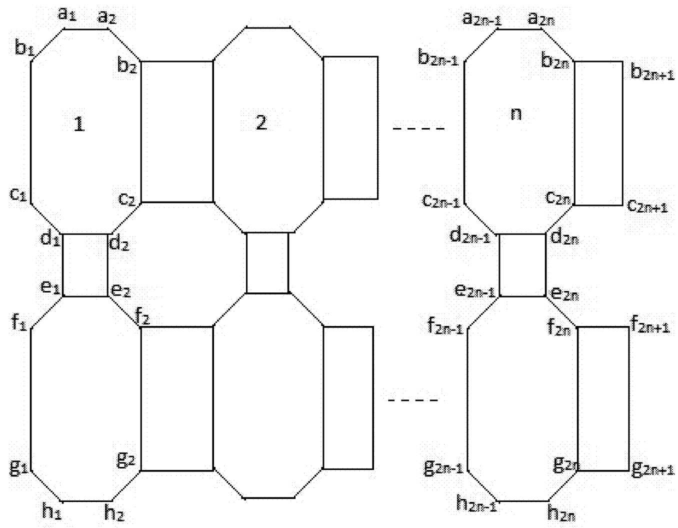

Figure 3.1

Theorem 3.1. *For $n \geq 3$, the Hosoya polynomial of $G(n, S_4)$ is*

$$\begin{aligned} H(G(n,S_4)) &= (22n+2)x + (34n-4)x^2 + (50n-14)x^3 \\ &\quad +(62n-26)x^4 + (66n-39)x^5 + (72n-56)x^6 \\ &\quad +(74n-75)x^7 + (70n-94)x^8 + (68n-112)x^9 \\ &\quad +(66n-126)x^{10} + \sum_{k=11}^{4n+1}(64n-(16k-36))x^k \\ &\quad +8x^{4n+2} + 2x^{4n+3} \end{aligned} \tag{2}$$

Proof. We use mathematical induction on n, $n \geq 3$. For $n = 3$, we find by direct calculation that

$$\begin{aligned} H(G(n,S_4)) &= 52 + 68x + 98x^2 + 136x^3 + 160x^4 + 159x^5 + 160x^6 \\ &\quad +147x^7 + 116x^8 + 92x^9 + 72x^{10} + 52x^{11} + 36x^{12} \\ &\quad +20x^{13} + 8x^{14} + 2x^{15}. \end{aligned}$$

Thus, (2) is true for $n = 3$. We assume that (2) is true for $n = r \geq 3$ and prove that it is true for $n = r + 1$. It is clear from Fig. 3.1 that

$$H(G(r+1,S_4)) = H(G(r,S_4)) + F(x),$$

where $F(x) = \sum_{i=1}^{16} H(w_i, G(r+1,S_4)) - (18x+20x^2+22x^3+20x^4+14x^5+12x^6+10x^7+4x^8)$. Here $w_1 = h_{2n+1}$, $w_2 = h_{2n+2}$, $w_3 = g_{2n+2}$, $w_4 = g_{2n+3}$, $w_5 = f_{2n+3}$, $w_6 = f_{2n+2}$, $w_7 = e_{2n+2}$, $w_8 = e_{2n+1}$, $w_9 = d_{2n+1}$, $w_{10} = d_{2n+2}$, $w_{11} = c_{2n+2}$, $w_{12} = c_{2n+3}$, $w_{13} = b_{2n+3}$, $w_{14} = b_{2n+2}$, $w_{15} = a_{2n+2}$, $w_{16} = a_{2n+1}$, (see Fig.3.1, for $n = r+1$). Then we find that

$$\begin{aligned} H(w_1, G(r+1,S_4)) &= 2x + 3x^2 + 5\sum_{k=3}^{5} x^k + 6x^6 + 7\sum_{k=7}^{8} x^k + 5x^9 \\ &\quad +4\sum_{k=10}^{4r+1} x^k + 3x^{4r+2} + 2x^{4r+3} + x^{4r+4} \\ &= H(w_{16}, G(r+1,S_4)), \end{aligned}$$

$$\begin{aligned} H(w_2, G(r+1,S_4)) &= 2x + 3x^2 + 4\sum_{k=3}^{5} x^k + 6x^6 + 7x^7 + 5\sum_{k=8}^{10} x^k \\ &\quad +4\sum_{k=11}^{4r+2} x^k + 3x^{4r+3} + 2x^{4r+4} + x^{4r+5} \\ &= H(w_{15}, G(r+1,S_4)), \end{aligned}$$

$$\begin{aligned}
H(w_3, G(r+1, S_4)) &= 3\textstyle\sum_{k=1}^{3} x^k + 4x^4 + 5x^5 + 6x^6 + 5x^7 + 4\sum_{k=8}^{4r+3} x^k \\
&\quad +3x^{4r+4} + 2x^{4r+5} + x^{4r+6} \\
&= H(w_{14}, G(r+1, S_4)),
\end{aligned}$$

$$\begin{aligned}
H(w_4, G(r+1, S_4)) &= 2\textstyle\sum_{k=1}^{3} x^k + 3x^4 + 4x^5 + 5x^6 + 6x^7 + 5x^8 \\
&\quad +4\textstyle\sum_{k=9}^{4r+4} x^k + 3x^{4r+5} + 2x^{4r+6} + x^{4r+7} \\
&= H(w_{13}, G(r+1, S_4)),
\end{aligned}$$

$$\begin{aligned}
H(w_5, G(r+1, S_4)) &= 2\textstyle\sum_{k=1}^{2} x^k + 3x^3 + 4x^4 + 5x^5 + 6x^6 + 5x^7 \\
&\quad +4\textstyle\sum_{k=8}^{4r+4} x^k + 3x^{4r+5} + x^{4r+6} \\
&= H(w_{12}, G(r+1, S_4)),
\end{aligned}$$

$$\begin{aligned}
H(w_6, G(r+1, S_4)) &= 3x + 4\textstyle\sum_{k=2}^{3} x^k + 5x^4 + 6x^5 + 5x^6 + 4\sum_{k=7}^{4r+3} x^k \\
&\quad +3x^{4r+4} + x^{4r+5} \\
&= H(w_{11}, G(r+1, S_4)),
\end{aligned}$$

$$\begin{aligned}
H(w_7, G(r+1, S_4)) &= 3x + 5x^2 + 7\textstyle\sum_{k=3}^{4} x^k + 5x^5 + 4\sum_{k=6}^{4r+2} x^k \\
&\quad +3x^{4r+3} + x^{4r+4} \\
&= H(w_{10}, G(r+1, S_4)),
\end{aligned}$$

$$\begin{aligned}
H(w_8, G(r+1, S_4)) &= 3x + 5x^2 + 8x^3 + 9x^4 + 6x^5 + 4\textstyle\sum_{k=6}^{4r+1} x^k \\
&\quad +3x^{4r+2} + x^{4r+3} \\
&= H(w_9, G(r+1, S_4)).
\end{aligned}$$

Thus

$$\begin{aligned}
H(G(r+1, S_4)) &= (22r+2)x + (34r-4)x^2 + (50r-14)x^3 \\
&\quad +(62r-26)x^4 + (66r-39)x^5 + (72r-56)x^6 \\
&\quad +(74r-75)x^7 + (70r-94)x^8 + (68r-112)x^9 \\
&\quad +(66r-126)x^{10} + \textstyle\sum_{k=11}^{4r+1}(64r-(16k-36))x^k \\
&\quad +8x^{4r+2} + 2x^{4r+3} + 22x + 34x^2 + 50x^3 + 62x^4 \\
&\quad +66x^5 + 72x^6 + 74x^7 + 70x^8 + 68x^9 + 66x^{10} \\
&\quad +64\textstyle\sum_{k=11}^{4r+1} x^k + 60x^{4r+2} + 50x^{4r+3} + 36x^{4r+4} \\
&\quad +20x^{4r+5} + 8x^{4r+6} + 2x^{4r+7}. \\
&= (22(r+1)+2)x + (34(r+1)-4)x^2 \\
&\quad +(50(r+1)-14)x^3 + (62(r+1)-26)x^4 \\
&\quad +(66(r+1)-39)x^5 + (72(r+1)-56)x^6 \\
&\quad +(74(r+1)-75)x^7 + (70(r+1)-94)x^8 \\
&\quad +(68(r+1)-112)x^9 + (66(r+1)-126)x^{10} \\
&\quad +\textstyle\sum_{k=11}^{4(r+1)+1}(64(r+1)-(16k-36))x^k \\
&\quad +8x^{4(r+1)+2} + 2x^{4(r+1)+3}.
\end{aligned}$$

Hence, Eqn. (2) is true for all n, $n \geq 3$. This completes the proof. □

Hosoya polynomials of $G(n, S_4)$ for $n = 1, 2$ are obtained as follows:

$$\begin{aligned}
H(G(1, S_4)) &= 24x + 30x^2 + 36x^3 + 36x^4 + 27x^5 + 20x^6 + 13x^7 + 4x^8, \\
H(G(2, S_4)) &= 46x + 64x^2 + 86x^3 + 98x^4 + 93x^5 + 88x^6 + 73x^7 + 46x^8 \\
&\quad +24x^9 + 10x^{10} + 2x^{11}.
\end{aligned}$$

Thus we can obtain $H(G(n, S_4))$ for all natural numbers n.

Theorem 3.2. *For $n \geq 3$, the Wiener index of $G(n, S_4)$ is given by*

$$W(G(n, S_4)) = (512n^3 + 864n^2 + 784n - 18)/3.$$

Proof. Wiener index can be obtained by taking derivative of $H(G(n, S_4))$ with respect to x and then substituting $x = 1$. The Wiener index of $H(G(1, S_4)) = 714$ and $H(G(2, S_4)) = 3034$. Hence we obtain the Wiener index for all natural numbers n. □

Now we consider another chain graph which will be denoted by $G(n, S_5)$, consisting of two rows of octagonal chains $G(n, S_1)$ where each row contains n octagons as shown in Fig. 3.2. This graph has $10n+4$ vertices and $13n+2$ edges.

Theorem 3.3. *For $n \geq 5$, the Hosoya polynomial of $G(n, S_5)$ is given by*

$$\begin{aligned} H(G(n,S_5)) &= (13n+2)x + (20n-2)x^2 + (30n-8)x^3 + (36n-18)x^4 \\ &\quad +(37n-30)x^5 + (40n-44)x^6 + (39n-58)x^7 \\ &\quad +(35n-69)x^8 + (34n-78)x^9 + (33n-87)x^{10} \\ &\quad +\textstyle\sum_{k=0}^{n-4}(33(n-k)-100)x^{3k+11} \\ &\quad +\textstyle\sum_{k=0}^{n-4}(34(n-k)-112)x^{3k+12} \\ &\quad +\textstyle\sum_{k=0}^{n-4}(33(n-k)-120)x^{3k+13} + 2x^{3n+2}. \end{aligned}$$

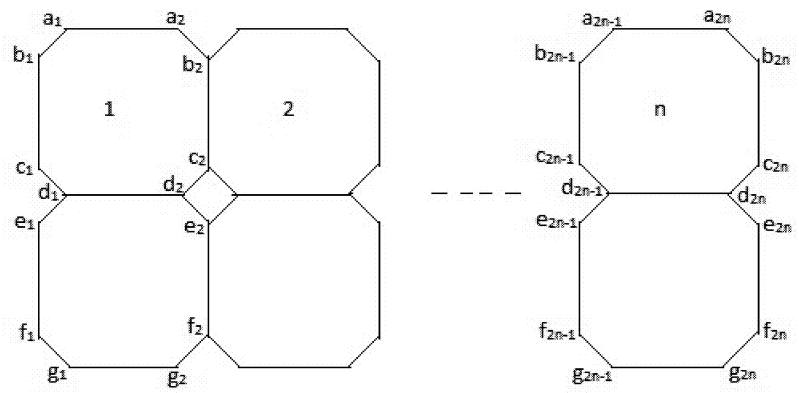

Figure 3.2

For $1 \leq n \leq 3$, the Hosoya polynomials of $G(n, S_5)$ are given by

$$\begin{aligned} H(G(1,S_5)) &= H(G(2,S_1)), \\ H(G(2,S_5)) &= 28x + 38x^2 + 52x^3 + 54x^4 + 44x^5 + 36x^6 + 20x^7 + 4x^8, \\ H(G(3,S_5)) &= 41x + 58x^2 + 82x^3 + 90x^4 + 81x^5 + 76x^6 + 59x^7 + 36x^8 \\ &\quad +24x^9 + 12x^{10} + 2x^{11}. \end{aligned}$$

By means of these values, we can obtain $H(n, S_5)$ for all natural numbers n.

Theorem 3.4. *For $n \geq 5$, the Wiener index of $G(n, S_5)$ is given by*

$$W(G(n, S_5)) = 50n^3 + 102n^2 + 139n - 2.$$

Proof. For $n \geq 5$, we have

$$\begin{aligned} W(G(n,S_5)) &= \frac{d}{dx}(H(G(n,S_5)))_{x=1} \\ &= (13n+1)+2(10n-2)+3(30n-8)+4(36n-18) \\ &\quad +5(37n-30)+6(40n-44)+7(39n-58)+8(35n-69) \\ &\quad +9(34n-78)+10(33n-87) \\ &\quad +\textstyle\sum_{k=0}^{n-4}(33(n-k)-100)(3k+11) \\ &\quad +\textstyle\sum_{k=0}^{n-4}(34(n-k)-112)(3k+12) \\ &\quad +\textstyle\sum_{k=0}^{n-4}(33(n-k)-120)(3k+13)+2(3n+2) \\ &= 50n^3+102n^2+139n-2. \end{aligned}$$

The above formula is valid for $n = 2, 3, 4$ and $W(G(1,S_5)) = W(G(2,S_5))$. Thus we can obtain $W(G(n,S_5))$ for all natural numbers. □

4. Conclusion

Wiener index was the first topological index defined in 1947 for determination of the boiling points of alkan isomers. Since then, many other topological indices have been defined and studied. Due to its pioneering role, many results related to the calculation of the Wiener index for graph classes, especially for the molecular graphs. In this work, we considered five classes of concatenated octachains and determined iteratively their Hosoya polynomials and by means of derivative, we calculated the Wiener indices of these chain classes.

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