The Expected Values of the Wiener Indices in the Random phenylene and spiro chains*

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Abstract. In this paper, we obtain some analytical expressions and give two simple formulae for the expected values of the Wiener indices of the random Phenylene and Spiro hexagonal chains.

Keywords: Wiener index; Random phenylene chain; Random spiro hexagonal chain

1 Introduction

In chemistry the topological indices of a molecular graph can provide some information on the chemical properties of the corresponding molecule. The first reported use of a topological index, the Wiener index, was by Wiener ([1]) in the study of paraffin boiling points. In the second half of the 20th century, the Wiener index was found to be correlated to many physicochemical properties and to have pharmacologic applications.

Spiro compounds are an important class of cycloalkanes in organic chemistry. A spiro union in spiro compounds is a linkage between two rings that consists of a single atom common to both rings and a free spiro union is a linkage that consists of the only direct union between the rings. Some results on energy, Merrifield-Simmons index, Hosoya index and Wiener index of the spiro chain was reported in ([2] [3]). Recently, Deng ([4] [5] [6]) gave the recurrences or explicit formulae for computing the Wiener index and Kirchhoff index of spiro chain. Huang and Kuang ([7]) obtained a simple exact formula for the expected value of the Kirchhoff index of a random spiro chain. The problem of calculation of the Wiener index of phenylenes

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was solved by Gutman ([8]). Recently, Chen ([9] [10])obtained two simple exact formulae for the expected values of the Merrifield-Simmons index and Wiener index of a random Phenylene chain.

In this paper, we obtain two explicit analytical expression for the expected values of the Wiener indices of a random phenylene chain $PH(n,p)$ and a random spiro chains $SPC(n,p_1,p_2)$,respectively.

2 Preliminaries

Let G be a graph with vertex set $\{v_1, v_2, \cdots, v_n\}$. The distance $d(v_r, v_s)$ between v_r and v_s in G is the length, or number of edges, of a shorest path in G that connects v_r and v_s. Under this definition $d(v_r, v_r) = 0$. The Wiener number of G is then defined by $W(G) = \sum_{r<s} d(v_r, v_s) = \frac{1}{2}\sum_{r=1}^{n}\sum_{s=1}^{n} d(v_r, v_s) = \frac{1}{2}\sum_{r=1}^{n} d(v_r|G)$, where $d(v_r|G)$ is the Wiener number of vertex v_r in G, defined by $d(v_r|G) = \sum_{s=1}^{n} d(v_r, v_s)$.

Phenylenes are a class of conjugated hydrocarbons composed of six- and four-membered rings, where the six-membered rings (hexagons) are adjacent only to four-membered rings, and every four-membered ring is adjacent to a pair of non-adjacent hexagons. If each six-membered ring of a phenylene is adjacent only to two four-membered rings, we say that it is a phenylene chain. Due to their aromatic and antiaromatic rings, phenylenes exhibit unique physico-chemical properties. In Fig. 1 some examples of phenylene chains are presented. The unique phenylene chains for $n = 1$ and $n = 2$ are shown in Fig. 1, where n is the number of hexagons in a phenylene chain.

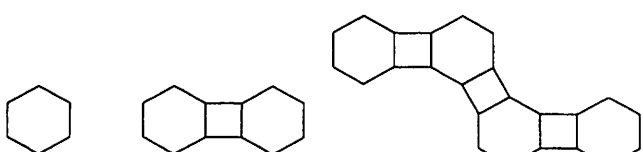

Fig. 1: Three examples of different phenylene chains.

More generally, a phenylene chain with n hexagons (see Fig.2) can be regarded as a phenylene chain PH_{n-1}, with $n-1$ hexagons to which a new terminal hexagon has been adjoined by a four-membered ring.

But, for $n \geq 3$, the terminal hexagon can be attached in three ways, which results in the local arrangements we describe as PH_{n+1}^1, PH_{n+1}^2, PH_{n+1}^3 (see Fig. 3).

A random phenylene chain $PH(n,p)$ with n hexagon is a phenylene chain obtained by stepwise addition of terminal hexagons. At each step $k(= 3, 4, \cdots, n)$ a random selection is made from one of the three possible

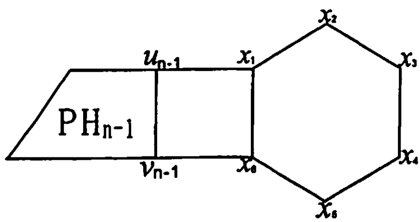

Fig. 2: A phenylene chain PH_n with n hexagons

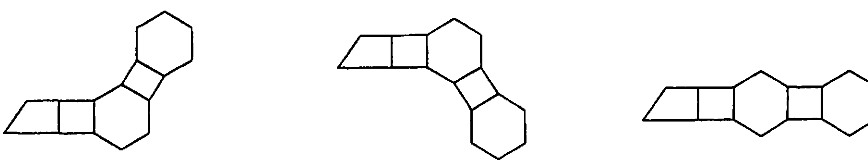

Fig. 3: The three types of local arrangements in phenylene chains.

constructions:(1)$PH_{k-1} \rightarrow PH_k^1$ with probability p, (2)$PH_{k-1} \rightarrow PH_k^2$ with probability p, (3)$PH_{k-1} \rightarrow PH_k^3$ with probability $1-2p$, where the probability p is constant, invariant to the step parameter k. That is, the process described is zeroth-order Markov process.

Also, a spiro chain SPC_n with n hexagons can be regarded as a spiro chain SPC_{n-1} with $n-1$ hexagons to which a new terminal hexagon has been adjoined (see Fig.4).

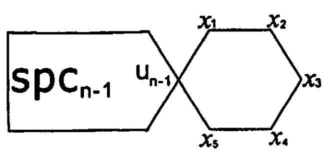

Fig. 4: A spiro chain SPC_n with n hexagons

For $n \geq 3$, the terminal hexagon can be attached in three ways, which results in the local arrangements we describe as SPC_{n+1}^1, SPC_{n+1}^2, SPC_{n+1}^3 (see Fig.5).

A random spiro chain $SPC(n, p_1, p_2)$ with n hexagon is a spiro chain obtained by stepwise addition of terminal hexagons. At each step $k(= 3, 4, \cdots, n)$ a random selection is made from one of the three possible constructions:(1)$SPC_{k-1} \rightarrow SPC_k^1$ with probability p_1, (2)$SPC_{k-1} \rightarrow$

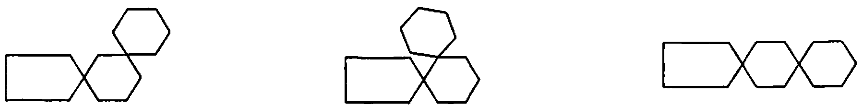

Fig. 5: A spiro chain SPC_n with n hexagons

SPC_k^2 with probability p_2, (3)$SPC_{k-1} \to SPC_k^3$ with probability $1-p_1-p_2$, where the probabilities p_1 and p_2 are constant, invariant to the step parameter k. That is, the process described is zeroth-order Markov process.

For a random phenylene chain $PH(n,p)$ and a random spiro chain $SPC(n,p_1,p_2)$, their Wiener indices are random variable. In this paper, we will obtain exact formulas for expected values $E(W(PH(n,p)))$ and $E(W(SPC(n,p_1,p_2)))$ of the Wiener indices in the random phenylene and spiro chains, respectively.

3 Main result:

In this section, we will give the expected values of the Wiener indices of random phenylene chains and spiro hexagonal chains. In [9], the authors have also consider the expected value of the Wiener index of random phenylene chains, but here we give exactly the expected value of the Wiener index of random phenylene chains in different method.

Theorem 1. *For $n \geq 1$, the expected value of the Wiener index of phenylene chain* $E(W(PH(n,p))) = (18-6p)n^3 + (9+18p)n^2 - 12pn$.

Proof: As described above, the phenylene chain PH_n can be regarded as a phenylene chain PH_{n-1}, with $n-1$ hexagons to which a new terminal hexagon has been adjoined by a four-membered ring. Suppose the terminal hexagon spans by $x_1, x_2, \cdots, x_6$, and the new edges are $u_{n-1}x_1$ and $v_{n-1}x_6$.(see Fig.2). Note that:
1. For any $v \in PH_{n-1}$,

$$d(x_1,v) = d(u_{n-1},v)+1, \qquad d(x_2,v) = d(u_{n-1},v)+2,$$
$$d(x_3,v) = d(u_{n-1},v)+3, \qquad d(x_4,v) = d(v_{n-1},v)+3,$$
$$d(x_5,v) = d(v_{n-1},v)+2, \qquad d(x_6,v) = d(v_{n-1},v)+1;$$

2. PH_{n-1} has $6(n-1)$ vertices;
3. $\sum_{i=1}^{6} d(x_k, x_i) = 9, \forall k \in \{1,2,3,4,5,6\}$. So we have :

$$d(x_1|PH_n) = d(u_{n-1}|PH_{n-1}) + 1 \times 6(n-1) + 9 \quad (1a);$$
$$d(x_2|PH_n) = d(u_{n-1}|PH_{n-1}) + 2 \times 6(n-1) + 9 \quad (1b);$$
$$d(x_3|PH_n) = d(u_{n-1}|PH_{n-1}) + 3 \times 6(n-1) + 9 \quad (1c);$$
$$d(x_4|PH_n) = d(v_{n-1}|PH_{n-1}) + 3 \times 6(n-1) + 9 \quad (1d);$$
$$d(x_5|PH_n) = d(v_{n-1}|PH_{n-1}) + 2 \times 6(n-1) + 9 \quad (1e);$$
$$d(x_6|PH_n) = d(v_{n-1}|PH_{n-1}) + 1 \times 6(n-1) + 9 \quad (1f);$$

and $W(PH_n) = W(PH_{n-1}) + 3d(u_{n-1}|PH_{n-1}) + 3d(v_{n-1}|PH_{n-1}) + 72n - 18 - \frac{1}{2}\sum_{i=1}^{6}\sum_{i=1}^{6} d(x_i, x_j)$, Then

$$W(PH_n) = W(PH_{n-1}) + 3d(u_{n-1}|PH_{n-1}) + 3d(v_{n-1}|PH_{n-1}) + 72n - 45 \quad (2).$$

For a random phenylene chain $PH(n,p)$, the distance number $d(u_n|PH(n,p))$ and $d(v_n|PH(n,p))$ are a random variable and we denote their expected values by $U_n = E(d(u_n \mid W(PH(n,p)))$ and $V_n = E(d(v_n \mid W(PH(n,p)))$ respectively.

case 1. $PH_n \to PH_{n+1}^1$. In this case, u_n coincides with the vertex labeled x_2 and v_n coincides with the vertex labeled x_3. Consequently, $d(u_n|PH_n)$ is given by eq.(1b) and $d(v_n|PH_n)$ is given by eq.(1c).

case 2. $PH_n \to PH_{n+1}^2$. In this case, u_n coincides with the vertex labeled x_4 and v_n coincides with the vertex labeled x_5. Consequently, $d(u_n|PH_n)$ is given by eq.(1d) and $d(v_n|PH_n)$ is given by eq.(1e).

case 3. $PH_n \to PH_{n+1}^3$. In this case, u_n coincides with the vertex labeled x_3 and v_n coincides with the vertex labeled x_4. Consequently, $d(u_n|PH_n)$ is given by eq.(1c) and $d(u_n|PH_n)$ is given by eq.(1d).

Since the above three cases occur in random phenylene chains with probabilities p and $1-2p$, we immediately obtain
$U_n = p[d(u_{n-1}|PH(n-1,p)) + 2 \times 6(n-1) + 9] + p[d(v_{n-1}|PH(n-1,p)) + 3 \times 6(n-1) + 9] + (1-2p)[d(u_{n-1}|PH(n-1,p)) + 3 \times 6(n-1) + 9]$;
$V_n = p[d(u_{n-1}|PH(n-1,p)) + 3 \times 6(n-1) + 9] + p[d(v_{n-1}|PH(n-1,p)) + 2 \times 6(n-1) + 9] + (1-2p)[d(v_{n-1}|PH(n-1,p)) + 3 \times 6(n-1) + 9]$;

By applying the expectation operator to the above equation, and noting that $E(U_n) = U_n$, we obtain $U_n = p(U_{n-1} + 12n - 3) + p(V_{n-1} + 18n - 9) + (1-2p)(U_{n-1} + 18n - 9)$; $V_n = p(U_{n-1} + 18n - 9) + p(V_{n-1} + 12n - 3) + (1-2p)(V_{n-1} + 18n - 9)$; It is easily transformed into:

$$U_n = (1-p)U_{n-1} + pV_{n-1} + (18-6p)n + 6p - 9;$$
$$V_n = (1-p)V_{n-1} + pU_{n-1} + (18-6p)n + 6p - 9;$$

The boundary condition is $U_1 = V_1 = E(d(u_1|PH(1,p))) = 1+1+2+2+3 = 9$, using the above recurrence relation and the boundary condition, we have

$$U_n = (9-3p)n^2 + 3pn. \quad (3)$$

A recurrence relation for the expected value of the Wiener number of a random phenylene chain can be obtained from eq. (2) and eq.(3), then we obtain

$$E(W(PH(n,p))) = E(W(PH(n-1,p))) + 6U_{n-1} + 72n - 45.$$

The boundary condition is $E(W(PH(1,p))) = 27$,using the above recurrence relation and the boundary condition, we have

$$E(W(PH(n,p))) = (18-6p)n^3 + (9+18p)n^2 - 12pn.$$

Theorem 2. *For $n \geq 1$, the expected value of the Wiener index of the spiro chain $SPC(n,p_1,p_2)$ is $E(W(SPC(n,p_1,p_2))) = \frac{1}{3}(45-15p_1-30p_2)n^3 + \frac{1}{2}(30p_1+60p_2+9)n^2 + (\frac{45}{6} - 10p_1 - 20p_2)n$.*

Proof: Note that the spiro chain SPC_n is obtained by attaching SPC_{n-1} a new terminal hexagon, we suppose that the terminal hexagon spans by $x_1, x_2, \cdots, x_6$, and the vertex x_1 is u_{n-1} (see Fig. 4). Note that:
1.For any $v \in SPC_{n-1}$,

$$\begin{aligned} &d(x_1,v) = d(u_{n-1},v)+1, && d(x_2,v) = d(u_{n-1},v)+2, \\ &d(x_3,v) = d(u_{n-1},v)+3, && d(x_4,v) = d(u_{n-1},v)+2, \\ &d(x_5,v) = d(u_{n-1},v)+1; && \end{aligned}$$

2.SPC_{n-1} has $5(n-1)+1 = 5n-4$ vertices; So we have :

$$\begin{aligned} d(x_1|SPC_n) &= d(u_{n-1}|SPC_{n-1}) + 1 \times (5n-4) + 8 \quad (4a); \\ d(x_2|SPC_n) &= d(u_{n-1}|SPC_{n-1}) + 2 \times (5n-4) + 7 \quad (4b); \\ d(x_3|SPC_n) &= d(u_{n-1}|SPC_{n-1}) + 3 \times (5n-4) + 6 \quad (4c); \\ d(x_4|SPC_n) &= d(u_{n-1}|SPC_{n-1}) + 2 \times (5n-4) + 7 \quad (4d); \\ d(x_5|SPC_n) &= d(u_{n-1}|SPC_{n-1}) + 1 \times (5n-4) + 8 \quad (4e) \end{aligned}$$

and $W(SPC_n) = W(SPC_{n-1}) + 6d(u_{n-1}|SPC_{n-1}) + 45n - \sum_{i=1}^{4}\sum_{j=i+1}^{5} d(x_i,x_j)$, Then

$$W(SPC_n) = W(SPC_{n-1}) + 6d(u_{n-1}|SPC_{n-1}) + 45n - 18. \quad (5)$$

For a random spiro chain $SPC(n,p_1,p_2)$, $d(u_n|SPC(n,p_1,p_2))$ is a random variable and we denote its expected value by $U_n = E(W(SPC(n,p_1,p_2)))$.

case 1. $SPC_n \to SPC^1_{n+1}$. In this case,u_n coincides with the vertex labeled x_2 or x_4. Consequently, $d(u_n|SPC_n)$ is given by eq. (4b) or (4d).

case 2. $SPC_n \to SPC^2_{n+1}$. In this case,u_n coincides with the vertex labeled x_1 or x_5. Consequently, $d(u_n|SPC_n)$ is given by eq. (4a) or (4e).

case 3. $SPC_n \to SPC^3_{n+1}$. In this case,u_n coincides with the vertex labeled x_3. Consequently, $d(u_n|SPC_n)$ is given by eq. (4c).

Since the above three cases occur in random spiro chains with probabilities p_1,p_2 and $1-p_1-p_2$, we immediately obtain
$U_n = p_1[d(u_{n-1}|SPC(n-1,p_1,p_2))+2\times(5n-4)+7]+p_2[d(v_{n-1}|SPC(n-1,p_1,p_2))+1\times(5n-4)+8]+(1-p_1-p_2)[d(u_{n-1}|SPC(n-1,p_1,p_2))+3\times(5n-4)+6]$;

By applying the expectation operator to the above equation, and noting that $E(U_n) = U_n$, we obtain $U_n = p_1(U_{n-1}+10n-1)+p_2(U_{n-1}+5n+4)+(1-p_1-p_2)(U_{n-1}+15n-6)$; It is easily transformed into:

$$U_n = U_{n-1}+(15-5p_1-10p_2)n+5p_1+10p_2-6;$$

The boundary condition is $U_1 = V_1 = E(d(u_1|SPC(1,p_1,p_2))) = 1+1+2+2+3 = 9$, using the above recurrence relation and the boundary condition, we have $U_n = \frac{1}{2}(15-5p_1-10p_2)n^2+\frac{1}{2}(5p_1+10p_2+3)n$. (6) A recurrence relation for the expected value of the Wiener number of a random spiro chain can be obtained from eq. (5) and eq.(6), then we obtain

$$E(W(SPC(n,p_1,p_2))) = E(W(SPC(n-1,p_1,p_2)))+6U_{n-1}+45n-18.$$

The boundary condition is $E(W(SPC(1,p_1,p_2))) = 27$,using the above recurrence relation and the boundary condition, we have
$E(W(SPC(n,p_1,p_2))) = \frac{1}{3}(45-15p_1-30p_2)n^3+\frac{1}{2}(30p_1+60p_2+9)n^2+(\frac{45}{6}-10p_1-20p_2)n$.

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