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*Original Scientific Paper*

# *The Gutman Index and Schultz Index in the Random Phenylene Chains*

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**ABSTRACT**

The Gutman index and Schultz index are two topological indices. In this paper, we first give exact formulae for the expected values of the Gutman index and Schultz index of random phenylene chains, and we will also get the average values of the Gutman index and Schultz index in phenylene chains.



## 1. INTRODUCTION

The study of topological properties of cyclic hydrocarbons have a long history, it promotes the research of hexagonal chain and quadrangle chain. So far, many achievements have been made, among which the research on mathematics mainly focuses on covering problem and related sorting problem and so on.

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The phenylene is composed of benzene and cyclobutadiene intercross, which makes it not only provides an excellent opportunity to detect the structural characteristics of various aromatic compounds, but also has potential practical USES, such as semiconductors, photoelectric emitters, etc. As a result, this has aroused great interest of many chemists and physicists and other scholars. Phenylene involves synthetic resin, plastic, rubber, capacitor, air quality, water quality, industrial dust and poison prevention technology, aerospace manufacturing, material protection, photosensitive materials, photograph technology and so on.

Topological indices are the graph invariants used in theoretical chemistry to encode molecules for the design of chemical compounds with given physicochemical properties or given pharmacological and biological activities [1]. The research on the topological indices of some special chemical chains and their application in chemistry has become a hot issue in chemical graph theory. In 1947, the Wiener index, introduced by Wiener, is the well-known topological index in a graph [2]. In 1994, the Gutman index and the Schultz index of a graph were introduced by Gutman, they are vertex-degree-based graph invariant [3]. Huang et al. obtained exact formulas for the expected values of the Kirchhoff indices of the random polyphenyl and spiro chains [4]. Recently, Geng er al. got the Kirchhoff indices and the number of spanning tree of möbius phenylene chain and cylinder phenylenes chain [5]. Deng et all. determined the first three maximal and minimal values of the Moster index among all hexagon chains with $h$ hexagons, and characterize the corresponding extremal graph by some transformations on hexagonal chains [6,7], and so on [8−13].

In this paper, we will present explicit formulae for the expected values of the Gutman index and Schultz index of random phenylene chains. We will also get the extremal values of these indices among all phenylene chains. At the end of this paper, we will give the average values of the Gutman index and Schultz index in phenylene chains.

## 2. PRELIMINARIES

In this section, All graph considered here are finite and simple. For a given graph $G = (V;E)$, the set of its vertices is denoted by $V$ and the set of its edges by $E$, $|V| = n$ and $|E| = m$. For a vertex $u \in V$, the degree of $u$, denote by $d_G(u)$(short for $d(u)$), is the number of vertices which are adjacent to $u$. The distance $d(u,v)$, is the length of a shortest path between $u$ and $v$.

Let $H$ be a cata-condensed hexagonal system. A hexagon $r$ has one neighbouring hexagon, then it is said to be terminal, and if it has three neighbouring hexagons, to be branched. A hexagon adjacent to exactly two other hexagons is a kink if $r$ possess two adjacent vertices of degree two, is linear otherwise. The dualist graph of $H$ consists of vertices corresponding to hexagons of $H$, two vertices are adjacent if and only if the corresponding hexagons have a common edge. Obviously, the dualist graph of $H$ is a tree. If $H$ has $n$ hexagons, then this tree has $n$ vertices and none of its vertices have degree greater than three. A cata-condensed hexagonal system with no branched hexagons is said to be a hexagonal chain. A hexagonal chain with no kink is said to be a linear chain.

Let $H$ be a cata-condensed hexagonal system with a least two hexagons. If we add quadrilaterals (face where boundary is a $4-$cycle) between all pair of adjacent hexagons of $H$, the obtained $G$ is called a phenylene. We call that $H$ is the hexagonal squeeze of $G$. A phenylene containing $n$ hexagons is called an $[n]-$phenylene. Clearly, there is one to one correspondence between a phenylene and its hexagonal squeeze, both possess the same number of hexagons. In addition, a phenylene with $n$ hexagons possess $n-1$ squares. The number of vertices of a phenylene and its hexagonal squeeze are $6n$ and $4n+2$, respectively. A phenylene chain with $n$ hexagons can be regarded as a phenylene chain $G_n$, see Figure 1.

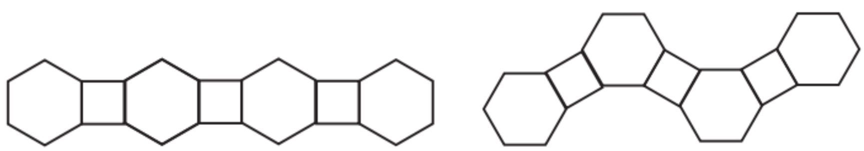

**Figure 1:** Examples of phenylene chain $G_4$.

A phenylene chain $G_{n+1}$ with $n+1$ hexagons can be regard as a phenylene chain $G_n$ with $n$ hexagons to which new terminal quadrilateral and hexagon have been adjoined, see Figure 2.

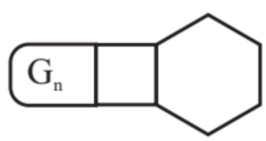


**Figure 2:** A phenylene chain $G_{n+1}$ with $n+1$ hexagons.

For $n \geq 2$, the terminal quadrilateral and hexagon can be attached in three ways, which results in the local arrangement we describe as $G_{n+1}^1, G_{n+1}^2, G_{n+1}^3$, see Figure 3.

A random phenylene chain $G_n(p, 1-2p, p)$ with $n$ hexagons is a phenylene chain obtained by stepwise addition of terminal quadrilateral and hexagon. At each step $k(k \geq 3)$, a random selection is made from one of the three possible constructions:

1. $G_{k-1} \rightarrow G_k^1$ with probability $p$,
2. $G_{k-1} \rightarrow G_k^2$ with probability $1-2p$,
3. $G_{k-1} \rightarrow G_k^3$ with probability $p$,

where the probability $p$ is a constant, satisfies the condition $0 \leq p \leq \frac{1}{2}$.

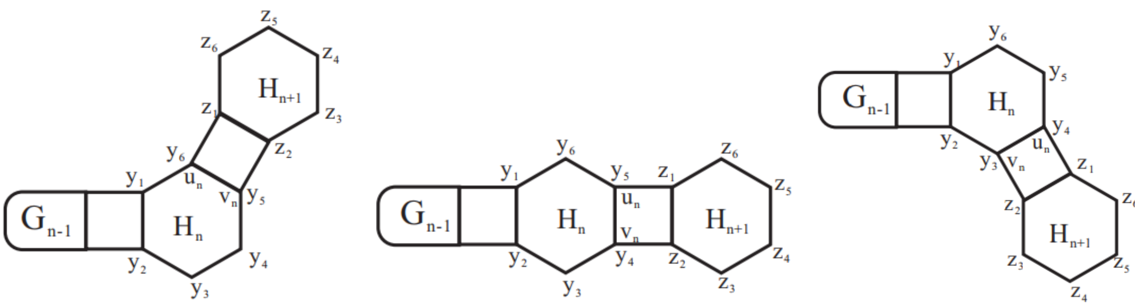


**Figure 3:** The three types of phenylene chains $G^1_{n+1}, G^2_{n+1}, G^3_{n+1}, respectively$.

Specially, the random phenylene chain $G_n(0,1,0)$ is the linear phenylene chain. Among all topological indices, the most well-known is the Wiener index [3], which is defined as

$$W(G) = \sum_{\{u,v\}\subseteq V(G)} d_G(u,v). \tag{1}$$

The Gutmn index is defined as

$$Gut(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u)d_G(v))d_G(u,v), \tag{2}$$

and the Schultz index is defined as

$$S(G) = \sum_{\{u,v\}\subseteq V(G)} (d_G(u) + d_G(v))d_G(u,v). \tag{3}$$

## 3. THE GUTMAN INDEX OF $G_n$

In this section, we consider the expected values $E(Gut(G_n))$ of Gutman index of a random phenylene chain $G_n$. As described above, the phenylene chain $G_{n+1}(p, 1-2p, p)$ is obtained at random by attaching $G_n$ a new quadrilateral and a new hexagon $H_{n+1}$ which is spanned by vertices $z_1, z_2, z_3, z_4, z_5, z_6$, from one of the three possible constructions (see Figure 3). The process is a zeroth-order Markov process. For $G_{n+1}(p, 1-2p, p)$, the Gutman index is random variable. For all $v \in G_n$, we have

$$\begin{aligned} &d(v,z_1) = d(v,u_n) + 1, d(v,z_2) = d(v,v_n) + 1, d(v,z_3) = d(v,v_n) + 2,\\ &d(v,z_4) = d(v,v_n) + 3, d(v,z_5) = d(v,u_n) + 3, d(v,z_6) = d(v,u_n) + 2. \end{aligned} \tag{4}$$

We also have

$$\begin{aligned} &\textstyle\sum_{i=1}^{6} d(z_i)d(z_i,z_1) = 19, \sum_{i=1}^{6} d(z_i)d(z_i,z_2) = 19, \sum_{i=1}^{6} d(z_i)d(z_i,z_3) = 21,\\ &\textstyle\sum_{i=1}^{6} d(z_i)d(z_i,z_4) = 23, \sum_{i=1}^{6} d(z_i)d(z_i,z_5) = 23, \sum_{i=1}^{6} d(z_i)d(z_i,z_6) = 21, \end{aligned} \tag{5}$$

and

$$\sum_{v\in V(G_n)} d_{G_{n+1}}(v) = 16n - 2. \qquad (6)$$

**Theorem 1** *Let $G_n$ be a random phenylene chain of length $n$. The expected value of the Gutman index of $G_n$ is*

$$E(Gut(G_n)) = \frac{1}{3}(384 - 128p)n^3 + (128p - 32)n^2 + \frac{1}{3}(36 - 256p)n. \qquad (7)$$

**Proof**. Let

$$Gut(G_{n+1}) = A + B + C, \qquad (8)$$

where

$$A = \sum_{\{u,v\}\subseteq G_n} d(u)d(v)d(u,v), \qquad (9)$$
$$B = \sum_{v\in G_n} \sum_{z_i\in H_{n+1}} d(v)d(z_i)d(v,z_i), \qquad (10)$$
$$C = \sum_{\{z_i,z_j\}\subseteq H_{n+1}} d(z_i)d(z_j)d(z_i,z_j), \qquad (11)$$

and

$$\begin{aligned}
A &= \sum_{\{u,v\}\subseteq G_n} d(u)d(v)d(u,v)\\
&= \sum_{\{u,v\}\subseteq G_n\backslash\{u_n,v_n\}} d(u)d(v)d(u,v) + \sum_{v\in G_n\backslash\{u_n,v_n\}} d(v)d(u_n)d(u_n,v)\\
&+ \sum_{v\in G_n\backslash\{u_n,v_n\}} d(v)d(v_n)d(v_n,v) + d(u_n)d(v_n)d(u_n,v_n)\\
&= \sum_{\{u,v\}\subseteq G_n\backslash\{u_n,v_n\}} d(u)d(v)d(u,v) + \sum_{v\in G_n\backslash\{u_n,v_n\}} d(v)(d_{G_n}(u_n)+1)d(u_n,v)\\
&+ \sum_{v\in G_n\backslash\{u_n,v_n\}} d(v)(d_{G_n}(v_n)+1)d(v_n,v) + (d_{G_n}(u_n)+1)(d_{G_n}(v_n)+1)d(u_n,v_n)\\
&= Gut(G_n) + \sum_{v\in G_n\backslash\{u_n,v_n\}} d(v)d(u_n,v) + \sum_{v\in G_n\backslash\{u_n,v_n\}} d(v)d(v_n,v) + 5\\
&= Gut(G_n) + \sum_{v\in G_n} d_{G_n}(v)d(u_n,v) + \sum_{v\in G_n} d_{G_n}(v)d(v_n,v) + 1,
\end{aligned}$$

$$\begin{aligned}
B &= \sum_{v\in G_n} \sum_{z_i\in H_{n+1}} d(v)d(z_i)d(v,z_i)\\
&= \sum_{v\in G_n} d(v)(3(d(v,u_n)+1) + 3(d(v,v_n)+1) + 2(d(v,u_n)+2)\\
&+ 2(d(v,v_n)+2) + 2(d(v,u_n)+3) + 2(d(v,v_n)+3))\\
&= 7\sum_{v\in G_n} d(v)d(v,u_n) + 7\sum_{v\in G_n} d(v)d(v,v_n) + 26\sum_{v\in G_n} d(v)\\
&= 7\sum_{v\in G_n\backslash\{u_n,v_n\}} d(v)d(v,u_n) + 7\sum_{v\in G_n\backslash\{u_n,v_n\}} d(v)d(v,v_n)\\
&+ 7d(v_n)d(v_n,u_n) + 7d(u_n)d(u_n,v_n) + 26(16n-2)\\
&= 7\sum_{v\in G_n} d_{G_n}(v)d(v,u_n) + 7\sum_{v\in G_n} d_{G_n}(v)d(v,v_n) + 14 + 26(16n-2)\\
&= 7\sum_{v\in G_n} d_{G_n}(v)d(v,u_n) + 7\sum_{v\in G_n} d_{G_n}(v)d(v,v_n) + 416n - 38,
\end{aligned}$$

and

$$\begin{aligned}
C &= \sum_{\{z_i,z_j\}\subseteq H_{n+1}} d(z_i)d(z_j)d(z_i,z_j)\\
&= \frac{1}{2}\sum_{i=1}^{6} d(z_i)(\sum_{i=1}^{6} d(z_j)d(z_i,z_j))\\
&= \frac{1}{2}(2\times 3\times 19 + 2\times 2\times 21 + 2\times 2\times 23)\\
&= 145.
\end{aligned}$$

Thus

$$Gut(G_{n+1}) = Gut(G_n) + 8\sum_{v\in G_n} d_{G_n}(v)d(v,u_n) \\ +8\sum_{v\in G_n} d_{G_n}(v)d(v,v_n) + 416n + 108. \quad (12)$$

Let $E_n^1 = E(\sum_{v\in G_n} d_{G_n}(v)d(v,u_n))$ and $E_n^2 = E(\sum_{v\in G_n} d_{G_n}(v)d(v,v_n))$, then we have

$$E(Gut(G_{n+1})) = E(Gut(G_n)) + 8E_n^1 + 8E_n^2 + 416n + 108. \quad (13)$$

We get $E_n^1$ and $E_n^2$ by considering three possible construction as described in Figure 3. If $G_n \to G_{n+1}^1$ with probability $p$, then $u_n = y_6, v_n = y_5$, we have

$$\sum_{v\in G_n} d_{G_n}(v)d(v,u_n) + \sum_{v\in G_n} d_{G_n}(v)d(v,v_n) = \sum_{v\in G_n} d_{G_n}(v)d(v,y_6) \\ +\sum_{v\in G_n} d_{G_n}(v)d(v,y_5),$$

If $G_n \to G_{n+1}^2$ with probability $1-2p$, then $u_n = y_5, v_n = y_4$, we have

$$\sum_{v\in G_n} d_{G_n}(v)d(v,u_n) + \sum_{v\in G_n} d_{G_n}(v)d(v,v_n) = \sum_{v\in G_n} d_{G_n}(v)d(v,y_5) \\ +\sum_{v\in G_n} d_{G_n}(v)d(v,y_4),$$

If $G_n \to G_{n+1}^3$ with probability $p$, then $u_n = y_4, v_n = y_3$, we have

$$\sum_{v\in G_n} d_{G_n}(v)d(v,u_n) + \sum_{v\in G_n} d_{G_n}(v)d(v,v_n) = \sum_{v\in G_n} d_{G_n}(v)d(v,y_4) \\ +\sum_{v\in G_n} d_{G_n}(v)d(v,y_3);$$

From above, we have

$$\begin{aligned}E_n^1 &= p\sum_{v\in G_n} d_{G_n}(v)d(v,y_6) + (1-2p)\sum_{v\in G_n} d_{G_n}(v)d(v,y_5) + p\sum_{v\in G_n} d_{G_n}(v)d(v,y_4)\\
&= p\big(\sum_{v\in G_{n-1}} d_{G_n}(v)(d(v,u_n)+2)+22\big) + p(\sum_{v\in G_{n-1}} d_{G_n}(v)(d(v,v_n)+3)+24)\\
&\quad +(1-2p)(\sum_{v\in G_{n-1}} d_{G_n}(v)(d(v,u_n)+3)+24)\\
&= p\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,u_n) + (1-2p)\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,u_n)\\
&\quad + p\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,v_n) + p\big(2\sum_{v\in G_{n-1}} d_{G_n}(v)+22\big)\\
&\quad + (1-2p)(3\sum_{v\in G_{n-1}} d_{G_n}(v)+24) + p(3\sum_{v\in G_{n-1}} d_{G_n}(v)+24)\\
&= p\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,u_n) + (1-2p)\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,u_n)\\
&\quad + p\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,v_n) + (48-16p)n + (16p-30),\end{aligned}$$

and

$$\begin{aligned}E_n^2 &= p\sum_{v\in G_n} d_{G_n}(v)d(v,y_5) + (1-2p)\sum_{v\in G_n} d_{G_n}(v)d(v,y_4) + p\sum_{v\in G_n} d_{G_n}(v)d(v,y_3)\\
&= p\big(\sum_{v\in G_{n-1}} d_{G_n}(v)(d(v,u_n)+3)+24\big)\\
&\quad + (1-2p)(\sum_{v\in G_{n-1}} d_{G_n}(v)(d(v,v_n)+3)+24)\\
&\quad + p(\sum_{v\in G_{n-1}} d_{G_n}(v)(d(v,v_n)+2)+22)\end{aligned}$$

$$= p\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,u_n) + (1-2p)\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,v_n)$$
$$+ p\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,v_n) + p(2\sum_{v\in G_{n-1}} d_{G_n}(v) + 22)$$
$$+ p\big(3\sum_{v\in G_{n-1}} d_{G_n}(v) + 24\big) + (1-2p)\big(3\sum_{v\in G_{n-1}} d_{G_n}(v) + 24\big)$$
$$= p\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,u_n) + (1-2p)\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,v_n)$$
$$+ p\sum_{v\in G_{n-1}} d_{G_n}(v)d(v,v_n) + (48-16p)n + (16p-30).$$

Then ,$E_n^1 + E_n^2 = E_{n-1}^1 + E_{n-1}^2 + (96-32p)n + (32p-60)$, the initial value is $E_1^1 + E_1^2 = \sum_{v\in G_1} d(v)d(v,u_1) + \sum_{v\in G_1} d(v)d(v,v_1) = 36$.

According to the calculation method of the progression, we have $E_n^1 + E_n^2 = (48-16p)n^2 + (16p-12)n$. So, we have $E(Gut(G_{n+1})) = E(Gut(G_n)) + 8E_n^1 + 8E_n^2 + 416n + 108 \quad = E(Gut(G_n)) + (384-128p)n^2 + (128p+320)n + 108$, the initial value is $E(Gut(G_1)) = 108$. Then, we have $E\big(Gut(G_n)\big) = \frac{1}{3}(384-128p)n^3 + (128p-32)n^2 + \frac{1}{3}(36-256p)n$. □

**Corollary 1** *The Gutman index of the linear phenylene chain $L_n$ is*

$$Gut(L_n) = 128n^3 - 32n^2 + 12n, \tag{14}$$

and the Gutman index of non-linear phenylene chain $P_n$ is

$$Gut(P_n) = \frac{320}{3}n^3 + 32n^2 - \frac{92}{3}n. \tag{15}$$

**Proof**. From (7), when $p = 0$ and $p = \frac{1}{2}$, respectively, we can get result. □

**Corollary 2** *Among all phenylene chain with $n(n \geq 3)$ hexagons, the graph with maximum Gutman index is linear chain, and the graph with minimum Gutman index is non-linear chain.*

**Proof**. Let $f(p) = E(Gut(G_n))$. Then,

$$f(p) = \frac{1}{3}(384-128p)n^3 + (128p-32)n^2 + \frac{1}{3}(36-256p)n$$
$$= (-\frac{128}{3}n^3 + 128n^2 - \frac{256}{3}n)p + 128n^3 - 32n^2 + 12n,$$

As $n \geq 3$, we have $\frac{\partial f}{\partial p} = -\frac{128}{3}n^3 + 128n^2 - \frac{256}{3}n < 0$. Note that $0 \leq p \leq \frac{1}{2}$, then $f(p) \leq 128n^3 - 32n^2 + 12n$, with equality if and only if $p = 0$. It is obvious that when $p = \frac{1}{2}$, $f(p)$ takes minimum values. □

## 4. THE SCHULTZ INDEX OF $G_n$

In this section, let $E(S(G_n))$ denote the expected value of Schultz index of the random phenylene chain $G_n$, we have

**Theorem 2** *Let $G_n$ be a random phenylene chain of length $n$. The expected value of the Schultz index of $G_n$ is*

$$E(S(G_n)) = (96 - 32p)n^3 + (12 + 96p)n^2 - 64pn. \tag{16}$$

**Proof**. Let

$$E(S(G_{n+1})) = A + B + C, \tag{17}$$

where

$$A = \sum_{\{u,v\}\subseteq G_n} \big(d(u) + d(v)\big)d(u,v), \tag{18}$$

$$B = \sum_{v\in G_n} \sum_{z_i\in H_{n+1}} \big(d(v) + d(z_i)\big)d(v,z_i), \tag{19}$$

$$C = \sum_{\{z_i,z_j\}\subseteq H_{n+1}} (d(z_i) + d(z_j))d(z_i,z_j), \tag{20}$$

and

$$\begin{aligned}
A &= \sum_{\{u,v\}\subseteq G_n} (d(u) + d(v))d(u,v) \\
&= \sum_{\{u,v\}\subseteq G_n\backslash\{u_n,v_n\}} (d(u) + d(v))d(u,v) + \sum_{v\in G_n\backslash\{u_n,v_n\}} (d(v) + d(u_n))d(u_n,v) \\
&+ \sum_{v\in G_n\backslash\{u_n,v_n\}} (d(v) + d(v_n))d(v_n,v) + (d(u_n) + d(v_n))d(u_n,v_n) \\
&= \sum_{\{u,v\}\subseteq G_n\{u_n,v_n\}} (d(u) + d(v))d(u,v) + \sum_{v\in G_n\{u_n,v_n\}} (d(v) \\
&+ d_{G_n}(u_n) + 1)d(u_n,v) + \sum_{v\in G_n\{u_n,v_n\}} \big(d(v) + d_{G_n}(v_n) + 1\big)d(v_n,v) \\
&+ (d_{G_n}(u_n) + d_{G_n}(v_n) + 2)d(u_n,v_n) \\
&= S(G_n) + \sum_{v\in G_n\backslash\{u_n,v_n\}} d(u_n,v) + \sum_{v\in G_n\backslash\{u_n,v_n\}} d(v_n,v) + 2 \\
&= S(G_n) + \sum_{v\in G_n} d(u_n,v) + \sum_{v\in G_n} d(v_n,v),
\end{aligned}$$

$$\begin{aligned}
B &= \sum_{v\in G_n} \sum_{z_i\in H_{n+1}} (d(v) + d(z_i))d(v,z_i) \\
&= \sum_{v\in G_n} d(v)(d(v,u_n) + 1 + d(v,v_n) + 1 + d(v,u_n) + 2 + d(v,v_n) + 2 \\
&+ d(v,u_n) + 3 + d(v,v_n) + 3) + \sum_{v\in G_n} (3(d(v,u_n) + 1) + 3(d(v,v_n) + 1) \\
&+ 2(d(v,u_n) + 2) + 2(d(v,v_n) + 2) + 2(d(v,u_n) + 3) + 2(d(v,v_n) + 3)) \\
&= 3\sum_{v\in G_n} d(v)d(v,u_n) + 3\sum_{v\in G_n} d(v)d(v,v_n) + 7\sum_{v\in G_n} d(v,v_n) \\
&+7\sum_{v\in G_n} d(v,u_n) + 12\sum_{v\in G_n} d(v) + \sum_{v\in G_n} 26 \\
&= 3\sum_{v\in G_n} d_{G_n}(v)d(v,u_n) + 3\sum_{v\in G_n} d_{G_n}(v)d(v,v_n) + 7\sum_{v\in G_n} d(v,v_n) \\
&+ 7\sum_{v\in G_n} d(v,u_n) + 6 + 12(16n - 2) + 26 \times 6n \\
&= 3\sum_{v\in G_n} d_{G_n}(v)d(v,u_n) + 3\sum_{v\in G_n} d_{G_n}(v)d(v,v_n) + 7\sum_{v\in G_n} d(v,v_n) \\
&+7\sum_{v\in G_n} d(v,u_n) + 348n - 18,
\end{aligned}$$

$$C = \sum_{\{z_i,z_j\}\subseteq H_{n+1}} (d(z_i) + d(z_j))d(z_i,z_j) = 9 \times (2 \times 3 + 4 \times 2) = 126.$$

Thus $S(G_{n+1}) = S(G_n) + 3\sum_{v\in G_n} d_{G_n}(v)d(v,u_n) + 3\sum_{v\in G_n} d_{G_n}(v)d(v,v_n) + 8\sum_{v\in G_n} d(v,u_n) + 348n + 108$. Let $E_n^1 + E_n^2 = E_n$, and $U_n^1 = \sum_{v\in G_n} d(v,u_n), U_n^2 = \sum_{v\in G_n} d(v,v_n)$, then we have

$$E(S(G_{n+1})) = E(S(G_n)) + 3E_n + 8U_n^1 + 8U_n^2 + 348n + 108. \tag{21}$$

We get $U_n^1$ and $U_n^2$ by considering three possible construction as described in Figure 3.

If $G_n \to G_{n+1}^1$ with probability $p$, then $u_n = y_6, v_n = y_5$, we have

$$\sum_{v\in G_n} d(v,u_n) + \sum_{v\in G_n} d(v,v_n) = \sum_{v\in G_n} d(v,y_6) + \sum_{v\in G_n} d(v,y_5),$$

If $G_n \to G_{n+1}^2$ with probability $1-2p$, then $u_n = y_5, v_n = y_4$, we have

$$\sum_{v\in G_n} d(v,u_n) + \sum_{v\in G_n} d(v,v_n) = \sum_{v\in G_n} d(v,y_5) + \sum_{v\in G_n} d(v,y_4),$$

If $G_n \to G_{n+1}^3$ with probability $p$, then $u_n = y_4, v_n = y_3$, we have

$$\sum_{v\in G_n} d(v,u_n) + \sum_{v\in G_n} d(v,v_n) = \sum_{v\in G_n} d(v,y_4) + \sum_{v\in G_n} d(v,y_3).$$

From above, we have

$$\begin{aligned}
U_n^1 &= p\sum_{v\in G_n} d(v,y_6) + (1-2p)\sum_{v\in G_n} d(v,y_5) + p\sum_{v\in G_n} d(v,y_4)\\
&= p(\sum_{v\in G_n} (d(v,u_{n-1}) + 2\times 6(n-1) + 9) + (1-2p)(\sum_{v\in G_n} (d(v,u_{n-1})\\
&\quad + 3\times 6(n-1) + 9) + p(\sum_{v\in G_n} (d(v,v_{n-1}) + 3\times 6(n-1) + 9)\\
&= p\sum_{v\in G_n} d(v,u_{n-1}) + (1-2p)\sum_{v\in G_n} d(v,u_{n-1}) + p\sum_{v\in G_n} (d(v,v_{n-1})\\
&\quad + (18-6p)n + (6p-9)
\end{aligned}$$

and

$$\begin{aligned}
U_n^2 &= p\sum_{v\in G_n} d(v,y_5) + (1-2p)\sum_{v\in G_n} d(v,y_4) + p\sum_{v\in G_n} d(v,y_3)\\
&= p(\sum_{v\in G_n} (d(v,u_{n-1}) + 3\times 6(n-1) + 9) + (1-2p)(\sum_{v\in G_n} (d(v,v_{n-1})\\
&\quad + 3\times 6(n-1) + 9) + p(\sum_{v\in G_n} (d(v,v_{n-1}) + 2\times 6(n-1) + 9)\\
&= p\sum_{v\in G_n} d(v,u_{n-1}) + (1-2p)\sum_{v\in G_n} d(v,v_{n-1}) + p\sum_{v\in G_n} (d(v,v_{n-1})\\
&\quad +(18-6p)n + (6p-9).
\end{aligned}$$

Then, $U_n^1 + U_n^2 = U_{n-1}^1 + U_{n-1}^2 + (36-12p)n + (12p-18)$, the initial value is $U_1^1 + U_1^2 = \sum_{v\in G_1} d(v,u_1) + \sum_{v\in G_1} d(v)d(v,v_1) = 18$. According to the calculation method of the progression, we have $U_n = U_n^1 + U_n^2 = (18-6p)n^2 + 6pn$.

From (14), we known $E_n = E_n^1 + E_n^2 = (48-16p)n^2 + (16p-12)n$. So, we have $E(S(G_{n+1})) = E(S(G_n)) + 3E_n + 8U_n + 348n + 108 = E(S(G_n)) + (288 - 96p)n^2 + (96p+312)n + 108$, the initial value is $E(S(G_1)) = 108$. Then, we have $E(S(G_n)) = (96-32p)n^3 + (12+96p)n^2 - 64pn$. □

**Corollary 3** *The Schultz index of the linear phenylene chain $L_n$ is*

$$S(L_n) = 96n^3 + 12n^2, \tag{22}$$

and the Schultz index of non-linear phenylene chain $P_n$ is

$$S(P_n) = 80n^3 + 60n^2 - 32n. \tag{23}$$

**Proof**. From (16), when $p = 0$ and $p = \frac{1}{2}$, respectively, we can get results. □

**Corollary 4** *Among all phenylene chain with $n (n \geq 3)$ hexagons, the graph with maximum Schultz index is linear chain, and the graph with minimum Schultz index is non-linear chain.*

**Proof**. Let

$$\begin{aligned} f(p) &= E(S(G_n)) \\ &= (96 - 32p)n^3 + (12 + 96p)n^2 - 64pn \\ &= (-32n^3 + 96n^2 - 64n)p + 96n^3 + 12n^2. \end{aligned}$$

As $n \geq 3$, we have $\frac{\partial f}{\partial p} = -32n^3 + 96n^2 - 64n < 0$. Note that $0 \leq p \leq \frac{1}{2}$, then $f(p) \leq 96n^3 + 12n^2$, with equality if and only if $p = 0$. It is obvious that when $p = \frac{1}{2}$, $f(p)$ takes minimum values. □

## 5. THE AVERAGE VALUES OF THE GUTMAN AND SCHULTZ INDICES OF RANDOM PHENYLENE CHAIN

In this section, we present the average values of the Gutman index and the Schultz index with respect to the set of all phenylene chains with $n$ hexagons. Let $\mathcal{G}_n$ is the set of all phenylene chain with $n$ hexagons. The average values of the Gutman index and the Schultz index with respect to $\mathcal{G}_n$ is

$$Gut_{avr}(\mathcal{G}_n) = \frac{1}{|\mathcal{G}_n|} \sum_{G \in \mathcal{G}_n} Gut(G),$$

$$S_{avr}(\mathcal{G}_n) = \frac{1}{|\mathcal{G}_n|} \sum_{G \in \mathcal{G}_n} S(G) \,.$$

**Theorem 3** *The average value of the Gutman index with respect to $\mathcal{G}_n$ is*

$$Gut_{avr}(\mathcal{G}_n) = \frac{1024}{9} n^3 + \frac{32}{3} n^2 - \frac{148}{9} n, \tag{24}$$

**Proof**. From (7), take $p = \frac{1}{3}$, we can get the result. □

**Theorem 4** *The average value of the Schultz index with respect to $\mathcal{G}_n$ is*

$$S_{avr}(\mathcal{G}_n) = \frac{256}{3} n^3 + 44n^2 - \frac{64}{3} n, \tag{25}$$

**Proof**. From (16), take $p = \frac{1}{3}$, we can get the result. □

From Corollary 1 and Corollary 3, we can get that the average values of the Gutman index and Schultz index with respect to $\{L_n, P_n\}$ are

$$\frac{Gut(L_n)+2Gut(P_n)}{3} = \frac{1024}{9}n^3 + \frac{32}{3}n^2 - \frac{148}{9}n, \tag{26}$$

and

$$\frac{S(L_n)+2S(P_n)}{3} = \frac{256}{3}n^3 + 44n^2 - \frac{64}{3}n. \tag{27}$$

This result show that the average values of the Gutman index and the Schultz index with respect to $\mathcal{G}_n$ are equal to the average values of the Gutman index and the Schultz index with respect to $\{L_n, P_n\}$, respectively.

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