symmetry

Article

Statistical Analyses of a Class of Random Cyclooctatetraene Chain Networks with Respect to Several Topological Properties

Chen Tao, Shengjun Tang * and Xianya Geng

School of Mathematics and Big Data, Anhui University of Science & Technology, Huainan 232001, China; 2022201444@aust.edu.cn (C.T.); 2012032@aust.edu.cn (X.G.)
* Correspondence: 2017021@aust.edu.cn

Abstract: In recent years, the research on complex networks has created a boom. The objective of the present paper is to study a random cyclooctatetraene chain whose graph-theoretic mathematical properties arose scientists' interests. By applying the concept of symmetry and probability theory, we obtain the explicit analytical expressions for the variances of Schultz index, multiplicative degree-Kirchhoff index Gutman index, and additive degree-Kirchhoff index of a random cyclooctatetraene chain with n octagons, which plays a crucial role in the research and application of topological indices.

Keywords: random cyclooctatetraene chain; Schultz index; multiplicative degree-Kirchhoff index; Gutman index; additive degree-Kirchhoff index

check for updates

Citation: Tao, C.; Tang, S.; Geng, X. Statistical Analyses of a Class of Random Cyclooctatetraene Chain Networks with Respect to Several Topological Properties. *Symmetry* **2023**, *15*, 1971. https://doi.org/10.3390/sym15111971

Academic Editors: Abel Cabrera Martínez and Alejandro Estrada-Moreno

Received: 19 September 2023
Revised: 17 October 2023
Accepted: 20 October 2023
Published: 24 October 2023

1. Introduction

In this paper, we just take finite and simple connected graphs into consideration, referring to [1] and the references cited therein. Chemistry is strongly linked to graph theory, and graph theory has been widely used in chemistry. In chemical graph theory, there are some alternatives between atoms that vertices represent the atoms and edges represent the covalent bonds. They are used to depict chemical compounds.

The molecular formula of a compound can represent different molecular structures and characteristics, but theoretical chemists are concerned with the physical and chemical properties of a compound and its relationship with the molecular formula of a compound. The physical and chemical properties of compounds are key areas of concern for theoretical chemists [2,3]. Polygonal chemicals have a wide diversity of molecular structures and their physical and chemical properties are becoming increasingly significant, which is referenced in [4–7].

There is no octagon in octagonal chains that has more than two cut-vertices, and such a octagonal chain is called a cyclooctatetraene chain. Cyclooctatetraene is the poster child for nonaromatic molecules. Cyclooctatetraene and its derivatives have fascinated chemists for a long time and have a wide range of applications in industry. Cyclooctatetraene differs from benzene in that it is not an aromatic hydrocarbon. It is chemically close to an unsaturated hydrocarbon. Not only can it be subjected to addition reactions, which is easily hydrogenated to form cyclooctane. It also oxidises and polymerises readily. A number of vital compounds of cyclooctatetraene can be served as substrates for the production of scientifically and commercially valuable materials. In this paper, we consider four kinds of indices of cyclooctatetraene chains with n octagons. We simply consider the situation starting from a vertex of a cyclooctatetraene chain, connecting an edge to another octagon. For more information about the cyclooctylene chain, we can refer to [8–11].

We give some basic notations. Set $G = (V_G, E_G)$ be a graph with vertices denoted V_G and edges denoted E_G. The number of edges in a graph G is denoted by $|E(G)|$. We claim that two vertices p and m are *adjacent* (or *neighbours*) if they are attached by an edge, which we will write as $p \sim m$. In G, the shortest length p, m-path among the paths between two vertices p and m is denoted as $d_G(p, m)$ (or simply $d(p, m)$). The Wiener index of G refers to the aggregate of distances between all the vertex pairs of G. It was created by H. Wiener in 1947 [12], that is

$$W(G) = \sum_{\{p,m\} \subseteq V_G} d(p,m). \tag{1}$$

The Wiener index is among the best studied, most understood, and most widely used molecular shape descriptors, and is based on graph theory, see [13–16].

A graph $G = (V_G, E_G)$ together with the weight function $\omega: V_G \to \mathbb{N}^+$ is known as a weighted graph [17] (G, ω). Let $\oplus$ denote one of the four arithmetic operations $+, -, \times, \div$ [18]. Consequently, the weighted Wiener index $W(G, \omega)$ is determined as

$$W(G,\omega) = \frac{1}{2} \sum_{p \in V_G} \sum_{m \in V_G} (\omega(p) \oplus \omega(m)) d(p,m). \tag{2}$$

Obviously, if $\omega \equiv 1$ and $\oplus$ denotes the operation $\times$, then $W(G,\omega) = W(G)$.
In case $\oplus$ represents the operation $\times$ and $\omega(\cdot) \equiv d_G(\cdot)$, then (2) is equivalent to [19]

$$Gut(G) = \frac{1}{2} \sum_{p \in V_G} \sum_{m \in V_G} (d_G(p) d_G(m)) d(p,m) = \sum_{\{p.m\} \subseteq V_G} (d_G(p) d_G(m)) d(p,m). \tag{3}$$

This is just the Gutman index. Research on possible chemical applications of the Gutman index and similar quantities and their theoretical study, for which polycyclic molecules are more difficult cases, see [20].

In case $\oplus$ represents the operation $+$ and $\omega(\cdot) \equiv d_G(\cdot)$, then (2) is equivalent to

$$S(G) = \frac{1}{2} \sum_{p \in V_G} \sum_{m \in V_G} (d_G(p) + d_G(m)) d(p,m) = \sum_{\{p.m\} \subseteq V_G} (d_G(p) + d_G(m)) d(p,m). \tag{4}$$

That's what the Schultz Index is all about. For additional articles on developing aspects of the topology indexes for [21–24], including mathematical properties, discrimination and applications, refer to [25].

In case of $a, b \in V(G)$, the resistance distance between a and b in G, is defined as the effective resistance between nodes a and b in the electrical network, where the nodes correspond to vertices of G and each edge of G is replaced by a resistor of unit resistance. The resistance distance between vertices a and b in G [26] is denoted as $r(a,b)$. For more detailed information, see [27–30]. It is the Kirchhoff index when the Wiener index is for non-trees, and this distance function is proposed by Klein and Randić [31], defined as

$$Kf(G) = \sum_{\{a,b\} \subseteq V_G} r(a,b). \tag{5}$$

For a description of the sum of eccentricity distances and the sum of eccentricity resistance-distances, refer to [32–36].

$Kf^*(G)$ was introduced by Chen and Zhang in 2007 [37] (see [38] for details), which is defined as

$$Kf^*(G) = \sum_{\{a,b\} \subseteq V_G} d(a) d(b) r(a,b), \tag{6}$$

Thus, the invariance of this graph is represented as

$$Kf^*(G) = 2|E_G| \sum_{i=2}^{n} \frac{1}{\lambda_i}, \tag{7}$$

from which $0 = \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n$ are the eigenvalues of $\ell(G)$. Moreover, $\ell(G)$ is the normalized Laplacian matrix of G, as proposed by Chung [39]. The normalized Laplacian index and multiplicative degree-Kirchhoff index play an essential application in mathematical chemistry and statistics. Research on these topics has attracted a wide range of attention from researchers.

$Kf^+(G)$ was introduced by Gutman, Feng and Yu in 2012 [40], which is defined as

$$Kf^+(G) = \sum_{\{a,b\}\subseteq V_G} (d(a)+d(b))r(a,b). \tag{8}$$

Probability properties are an important component of chemical graphs, which can more broadly describe the topological properties and structures of chemical graphs. In this paper, we focus on the cyclooctatetraene chain G_n with n octagons, which is formed as follows.

Firstly, G_1 is an octagon and G_2 is the graph with two octagons, as shown in Figure 1.

Secondly, by appending a new terminal octagon H_{n+1} to G_n, the random cyclooctatetraene chain G_{n+1} with n octagons can be constructed. We illustrates this process in Figure 2. As demonstrated in Figure 3, we can append the terminal octagon H_{n+1} to G_n with four methods and indicate the generated figures with G^1_{n+1}, G^2_{n+1}, G^3_{n+1}, and G^4_{n+1}, respectively.

At each step, randomly pick one of the following possible outcomes:

- p_1 is the probability that $G_n \to G^1_{n+1}$;
- p_2 is the probability that $G_n \to G^2_{n+1}$
- p_3 is the probability that $G_n \to G^3_{n+1}$
- $p_4 = 1 - p_1 - p_2 - p_3$ is the probability that $G_n \to G^4_{n+1}$.

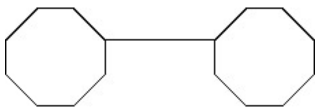

Figure 1. Graph G_2

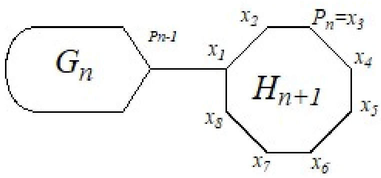

Figure 2. The construction of G_{n+1} from G_n and H_{n+1}.

We consider four random variables Z^1_n, Z^2_n, Z^3_n, and Z^4_n for our choice. When $i = 1, 2, 3, 4$, in case our selection is G^i_{n+1}, we have $Z^i_n = 1$; otherwise, $Z^i_n = 0$, and we can easily derive that

$$P(Z^i_n = 1) = p_i, P(Z^i_n = 0) + P(Z^i_n = 1) = 1 \tag{9}$$

and $Z^1_n + Z^2_n + Z^3_n + Z^4_n = 1$.

Through the above process, we get a random cyclooctatetraene chain $G_n(p_1, p_2, p_3, p_4)$. We always abbreviate $G_n(p_1, p_2, p_3, p_4)$ to G_n. All of $S(G_n)$, $Kf^*(G_n)$, $Gut(G_n)$and $Kf^+(G_n)$ are random variables in probability by noting that G_n is a random graph. From a probabilistic point of view, a natural question arises: when n is big enough, will the distribution of $S(G_n)$, $Kf^*(G_n)$, $Gut(G_n)$ and $Kf^+(G_n)$ look like a probability distribution or not.

In this paper, we make researches on $S(G_n)$, $Kf^*(G_n)$, $Gut(G_n)$ and $Kf^+(G_n)$. There is a huge amount of relevant literature. For random polyphenylene chain, J.I. Zhang, X.H. Peng, H.I. Chen [18] established the limiting behaviours of $S(G_n)$, $Kf^*(G_n)$, $Gut(G_n)$ and $Kf^+(G_n)$. Here it is natural and interesting to consider limiting behaviours of $S(G_n)$, $Kf^*(G_n)$, $Gut(G_n)$ and $Kf^+(G_n)$ for random cyclooctatetraene chain. In this paper, by applying the concept of symmetry and probability theory, we derive definite analytical expressions for the variance of the Schultz index, multiplicative degree-Kirchhoff index, Gutman index and additive degree-Kirchhoff index of a random cyclooctatetraene chain with n octagons, which plays a crucial role in the research and application of topological indices.

In this paper, in order to better describe the probability properties of cyclooctylene chain, we propose the following hypothesis.

Hypothesis 1. *We choose to attach the new terminal octagon H_{n+1} to G_n, where $n = 2, 3, ...$, and it is random and independent. More precisely, a range of random variables $Z_n^1, Z_n^2, Z_n^3, Z_{n}^{4}{}_{n=2}^{\infty}$ is independent and has the same law (9). With regard to some $i \in 1, 2, 3$, $0 < p_i < 1$ is obvious. Based on Hypothesis 1, we present analytical expressions for the variances of $S(G_n)$, $Kf^*(G_n)$, $Gut(G_n)$ and $Kf^+(G_n)$.*

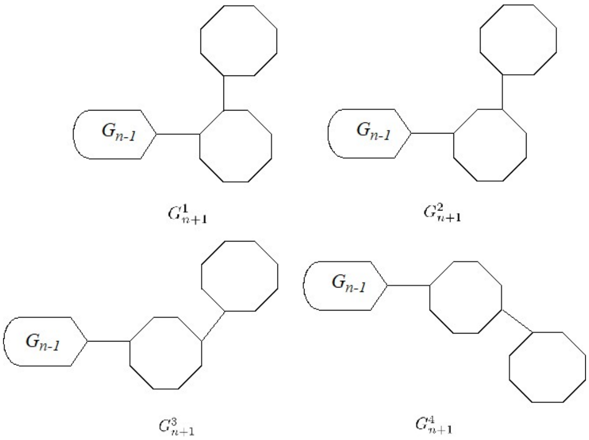

Figure 3. Four ways to attach the new terminal octagon H_{n+1} to G_n.

2. The Variances for the Gutman Index and Schultz Index of a Random Cyclooctatetraene Chain

For all G_n, the Gutman index and Schultz index of a random cyclooctatetraene chain are random variables. We are going to take the variances of $Gut(G_n)$ and $S(G_n)$ into consideration in this section. Actually, G_{n+1} is G_n connected by an edge to a new terminal octagon H_{n+1}, where H_{n+1} is extended by vertices x_1, x_2, x_3, x_4, x_5, x_6, x_7, and x_8, and $p_n x_1$ is the new edge; see Figure 2. On the one hand, for all $m \in V_{G_n}$,

$$d(x_1, m) = d(p_n, m) + 1,\ \ d(x_2, m) = d(p_n, m) + 2,\ \ d(x_3, m) = d(p_n, m) + 3,\ \ d(x_4, m) = d(p_n, m) + 4, \tag{10}$$

$$d(x_5, m) = d(p_n, m) + 5,\ \ d(x_6, m) = d(p_n, m) + 4,\ \ d(x_7, m) = d(p_n, m) + 3,\ \ d(x_2, m) = d(p_n, m) + 2, \tag{11}$$

$$\sum_{m \in V_{G_n}} d_{G_{n+1}}(m) = 18n - 1. \tag{12}$$

on the other hand, for all $t \in \{1, 2, 3, 4, 5, 6, 7, 8\}$

$$\sum_{t=1}^{8} d(x_t)d(x_1, x_t) = 32,\ \ \sum_{t=1}^{8} d(x_t)d(x_2, x_t) = 33,\ \ \sum_{t=1}^{8} d(x_t)d(x_3, x_t) = 34,\ \ \sum_{t=1}^{8} d(x_t)d(x_4, x_t) = 35, \tag{13}$$

$$\sum_{t=1}^{8} d(x_t)d(x_5, x_t) = 36,\ \ \sum_{t=1}^{8} d(x_t)d(x_6, x_t) = 35,\ \ \sum_{t=1}^{8} d(x_t)d(x_7, x_t) = 34,\ \ \sum_{t=1}^{8} d(x_t)d(x_8, x_t) = 33. \tag{14}$$

In [41] Theorem 1, the author proves that

$$\begin{aligned} E(Gut(G_n)) =& (270 - 162p_1 - 108p_2 - 54p_3)n^3 + (486p_1 + 324p_2 + 162p_3 - 90)n^2 \\ & + (77 - 324p_1 - 216p_2 - 108p_3)n - 1. \end{aligned}$$

where $E(Gut(G_n)$ is the mathematical expectations of $Gut(G_n)$.

We now present the first main result of this section.

Theorem 1. *The results are as follows, if Hypothesis 1 holds. As to the random cyclooctatetraene chain G_n, the variance of Gutman index $Gut(G_n)$, computed as*

$$Var(Gut(G_n)) = \frac{1}{30}(\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 \\ + (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)).$$

where

$$\begin{aligned} \sigma^2 =& 648^2 p_1 + 972^2 p_2 + 1296^2 p_3 + 1620^2 p_4 - (648p_1 + 972p_2 + 1296p_3 + 1620p_4)^2 \\ \tilde{\sigma}^2 =& 90^2 p_1 + 414^2 p_2 + 738^2 p_3 + 1062^2 p_4 - (90p_1 + 414p_2 + 738p_3 + 1062p_4)^2 \\ r =& 648 \cdot 90 \cdot p_1 + 972 \cdot 414 \cdot p_2 + 1296 \cdot 738 \cdot p_3 + 1620 \cdot 1062 \cdot p_4 \\ & - (648p_1 + 972p_2 + 1296p_3 + 1620p_4) \cdot (90p_1 + 414p_2 + 738p_3 + 1062p_4) \end{aligned}$$

Proof. Let

$$A_n := 18 \sum_{m \in V_{G_n}} d(m)d(p_n, m).$$

then, by (5.1) of [41], we obtain

$$Gut(G_{n+1}) = Gut(G_n) + A_n + 882n + 239. \tag{15}$$

□

Recalling from Section 1 that Z_n^1, Z_n^2, Z_n^3, and Z_n^4 are random variables, this indicates our option in constructing G_{n+1} from G_n. We have four equalities as follows:
Equality 1.

$$A_n Z_n^1 = (A_{n-1} + 648n - 90)Z_n^1.$$

If $Z_n^1 = 0$, the equality mentioned above is evident. Thus, we only have to regard the case $Z_n^1 = 1$, which means that $G_n \longrightarrow G_{n+1}^1$. In this view, p_n (of G_n) is coincident with the vertex labeled x_2 or x_8 (of H_n), see Figure 4. In this scenario, A_n turns into

$$\begin{aligned} 18 \sum_{m \in V_{G_n}} d(m)d(x_2, m) &= 18 \sum_{m \in V_{G_{n-1}}} d(m)d(x_2, m) + 18 \sum_{m \in V_{H_n}} d(m)d(x_2, m) \\ &= 18 \sum_{m \in V_{G_{n-1}}} d(m)(d(m, p_{n-1}) + d(x_2, p_{n-1})) + 18 \times 33 \\ &= 18 \sum_{m \in V_{G_{n-1}}} d(m)(d(m, p_{n-1}) + 2) + 18 \times 33 \\ &= A_{n-1} + 36 \sum_{m \in V_{G_{n-1}}} d(m) + 594 \\ &= A_{n-1} + 36(18n - 19) + 594 \\ &= A_{n-1} + 648n - 90, \end{aligned}$$

In the foregoing, we utilised (10)–(12). As a result, we arrive at the required equivalence conclusion.
Equality 2.

$$A_n Z_n^2 = (A_{n-1} + 972n - 414)Z_n^2.$$

As in the proof of Equality 1, we only have to regard the case $Z_n^2 = 1$, which is $G_n \longrightarrow G_{n+1}^2$. The proof process is analogous, and we leave out the details.

Equality 3.

$$A_n Z_n^3 = (A_{n-1} + 1296n - 738) Z_n^3$$

We have to regard the case $Z_n^3 = 1$, which is $G_n \longrightarrow G_{n+1}^3$. The proof is the same as Equality 1 and we omit the details.

Equality 4.

$$A_n Z_n^4 = (A_{n-1} + 1620n - 1062) Z_n^4$$

We have to regard the case $Z_n^4 = 1$, which is $G_n \longrightarrow G_{n+1}^4$. The proof process is also analogous, and we leave out the details.

Recalling that $Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4 = 1$, according to the above discussion, it holds that

$$\begin{aligned}
A_n &= A_n(Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4) \\
&= (A_{n-1} + 648n - 90)Z_n^1 + (A_{n-1} + 972n - 414)Z_n^2 + (A_{n-1} + 1296n - 738)Z_n^3 + (A_{n-1} + 1620n - 1062)Z_n^4 \\
&= A_{n-1} + (648Z_n^1 + 972Z_n^2 + 1296Z_n^3 + 1620Z_n^4)n - (90Z_n^1 + 414Z_n^2 + 738Z_n^3 + 1062Z_n^4) \\
&= A_{n-1} + n \cdot U_n - V_n.
\end{aligned}$$

For each n, it indicates that $U_n = 648Z_n^1 + 972Z_n^2 + 1296Z_n^3 + 1620Z_n^4$, $V_n = 90Z_n^1 + 414Z_n^2 + 738Z_n^3 + 1062Z_n^4$.

Therefore, by (15) we obtain

$$\begin{aligned}
Gut(G_n) &= Gut(G_1) + \sum_{t=1}^{n-1} A_t + \sum_{t=1}^{n-1}(882t + 239) \\
&= Gut(G_1) + \sum_{t=1}^{n-1}\Big(\sum_{q=1}^{t-1}(A_{q+1} - A_q) + A_1\Big) + \sum_{t=1}^{n-1}(882t + 239) \\
&= Gut(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}(A_{q+1} - A_q) + (n-1)A_1 + \sum_{t=1}^{n-1}(882t + 239) \\
&= Gut(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}((q+1)U_{q+1} - V_{q+1}) + (n-1)A_1 + \sum_{t=1}^{n-1}(882t + 239) \\
&= Gut(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}((q+1)U_{q+1} - V_{q+1}) + O(n^2)
\end{aligned}$$

where $O(n^2)$ representing high-order infinitesimal of n^2.

By direct calculation, one sees that $Var(U_q) = \sigma^2$, $Var(V_q) = \tilde{\sigma}^2$, and $Cov(U_q, V_q) = r$, where for any two random variables X and Y, $Cov(X, Y) = E(XY) - E(X) \cdot E(Y)$. Based on the nature of the variance and the order in which the sums are exchanged, it can be concluded that

$$\begin{aligned}
Var(Gut(G_n)) &= Var(\sum_{t=1}^{n-1}\sum_{q=1}^{t-1}((q+1)U_{q+1}-V_{q+1})) \\
&= Var(\sum_{q=1}^{n-2}\sum_{t=q+1}^{n-1}((q+1)U_{q+1}-V_{q+1})) \\
&= Var(\sum_{q=1}^{n-2}((q+1)U_{q+1}-V_{q+1})(n-q-1)) \\
&= \sum_{q=1}^{n-2}(n-q-1)^2 Var((q+1)U_{q+1}-V_{q+1}) \\
&= \sum_{q=1}^{n-2}(n-q-1)^2 Cov((q+1)U_{q+1}-V_{q+1},(q+1)U_{q+1}-V_{q+1}) \\
&= \sum_{q=1}^{n-2}(n-q-1)^2((q+1)^2 Cov(U_{q+1},U_{q+1})-2(q+1)Cov(U_{q+1},V_{q+1})+Cov(V_{q+1},V_{q+1})) \\
&= \sum_{q=1}^{n-2}(n-q-1)^2((q+1)^2\sigma^2-2(q+1)r+\tilde{\sigma}^2).
\end{aligned}$$

By means of computational, ad hoc tools, the above equality gives the required results, $Var(Gut(G_n))$.

Now, we discuss the variance of the Schultz index.

By Theorem 2.3 of [41], we have

$$\begin{aligned}
E(S(G_n)) =& (240-144p_1-96p_2-48p_3)n^3+(432p_1+288p_2+144p_3-40)n^2 \\
&+(56-288p_1-192p_2-96p_3)n.
\end{aligned}$$

After that we illustrate our results.

Theorem 2. *Supposing that Hypothesis 1, then the following results are true. As to the random cyclooctatetraene chain G_n, the variance of Schultz index $S(G_n)$, computed as*

$$\begin{aligned}
Var(S(G_n)) =& \frac{1}{30}(\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 \\
&+(-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)).
\end{aligned}$$

where

$$\begin{aligned}
\sigma^2 =& 576^2 p_1 + 864^2 p_2 + 1152^2 p_3 + 1440^2 p_4 - (576p_1 + 864p_2 + 1152p_3 + 1440p_4)^2 \\
\tilde{\sigma}^2 =& 40^2 p_1 + 328^2 p_2 + 616^2 p_3 + 904^2 p_4 - (40p_1 + 328p_2 + 616p_3 + 904p_4)^2 \\
r =& 576\cdot 40\cdot p_1 + 864\cdot 328\cdot p_2 + 1152\cdot 616\cdot p_3 + 1440\cdot 904\cdot p_4 \\
&-(576p_1 + 864p_2 + 1152p_3 + 1440p_4)\cdot(40p_1 + 328p_2 + 616p_3 + 904p_4)
\end{aligned}$$

Proof. By [41] (5.2), we obtain

$$S(G_{n+1}) = S(G_n) + 18\sum_{m\in V_{G_n}} d(p_n,m) + 8\sum_{m\in V_{G_n}} d(m)d(p_n,m) + 824n + 248. \quad (16)$$

and

$$B_n := \sum_{m\in V_{G_n}} (18 + 8d(m))d(p_n,m).$$

$$S(G_{n+1}) = S(G_n) + B_n + 824n + 248.$$

□

After similar discussions, we have four equalities as follows:

Equality 1.

$$B_n Z_n^1 = (B_{n-1} + 576n - 40) Z_n^1$$

If $Z_n^1 = 0$, the equality mentioned above is evident, so we only have to regard the case $Z_n^1 = 1$, which means that $G_n \longrightarrow G_{n+1}^1$. In this view, p_n (of G_n) is coincident with the vertex labeled x_2 or x_8 (of H_n), see Figure 4. In this scenario, B_n turns into

$$\begin{aligned}
B_n &= \sum_{m \in V_{G_n}} (18 + 8d(m)) d(x_2, m) \\
&= \sum_{m \in V_{G_{n-1}}} (18 + 8d(m)) d(x_2, m) + \sum_{m \in V_{H_n}} (18 + 8d(m)) d(x_2, m) \\
&= \sum_{m \in V_{G_{n-1}}} (18 + 8d(m))(d(p_{n-1}, m) + 2) + 18 \times 16 + 8 \times 33 \\
&= \sum_{m \in V_{G_{n-1}}} (18 + 8d(m)) d(p_{n-1}, m) + 2 \sum_{m \in V_{G_{n-1}}} (18 + 8d(m)) + 18 \times 16 + 8 \times 33 \\
&= \sum_{m \in V_{G_{n-1}}} (18 + 8d(m)) d(p_{n-1}, m) + 2(18 \times 8(n-1) + 8 \times (18(n-1) - 1)) + 18 \times 16 + 8 \times 33 \\
&= B_{n-1} + 2(288n - 296) + 552 \\
&= B_{n-1} + 576n - 40
\end{aligned}$$

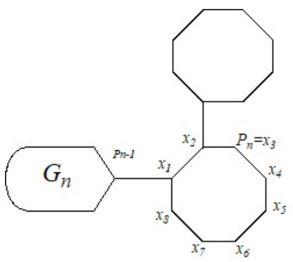

Figure 4. $G_n \to G_{n+1}^1$.

In the foregoing, we utilised (10)–(12). As a result, we arrive at the required equivalence conclusion.

Equality 2.

$$B_n Z_n^2 = (B_{n-1} + 864n - 328) Z_n^2$$

As in the proof of Equality 1, we only have to regard the case $Z_n^2 = 1$, which is $G_n \longrightarrow G_{n+1}^2$. The proof process is analogous, and we leave out the details.

Equality 3.

$$B_n Z_n^3 = (B_{n-1} + 1152n - 616) Z_n^3$$

We have to regard the case $Z_n^3 = 1$, which is $G_n \longrightarrow G_{n+1}^3$. The proof is the same as Equality 1 and we omit the details.

Equality 4.

$$B_n Z_n^4 = (B_{n-1} + 1440n - 904) Z_n^4$$

We have to regard the case $Z_n^4 = 1$, which is $G_n \longrightarrow G_{n+1}^4$. The proof process is also analogous, and we leave out the details.

Recalling that $Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4 = 1$, according to the above discussion, it holds that

$$\begin{aligned} B_n &= B_n(Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4) \\ &= B_{n-1} + n \cdot U_n - V_n \end{aligned}$$

where for each n, $U_n = 576Z_n^1 + 864Z_n^2 + 1152Z_n^3 + 1440Z_n^4$, $V_n = 40Z_n^1 + 328Z_n^2 + 616Z_n^3 + 904Z_n^4$.

Therefore, by (15)

$$\begin{aligned} S(G_n) &= S(G_1) + \sum_{t=1}^{n-1} B_t + \sum_{t=1}^{n-1}(824t + 248) \\ &= S(G_1) + \sum_{t=1}^{n-1}(\sum_{q=1}^{t-1}(B_{q+1} - B_q) + B_1) + \sum_{t=1}^{n-1}(824t + 2489) \\ &= S(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}(B_{q+1} - B_q) + (n-1)B_1 + \sum_{t=1}^{n-1}(824t + 248) \\ &= S(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}((q+1)U_{q+1} - V_{q+1}) + (n-1)B_1 + \sum_{t=1}^{n-1}(824t + 248) \\ &= S(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}((q+1)U_{q+1} - V_{q+1}) + O(n^2). \end{aligned}$$

If we replace $Gut(G_n)$ from the proof of Theorem 1 by $S(G_n)$, the rest of the proof of this theorem is the same as the proof of Theorem 1, and therefore the details are omitted.

3. The Variances of Multiplicative and Additive Degree-Kirchhoff Indices of a Random Cyclooctatetraene Chain

In the section, we talk about the variances for the multiplicative degree-Kirchhoff index $Kf^*(G_n)$ and the additive degree-Kirchhoff index $Kf^+(G_n)$. For a random cyclooctatetraene chain G_n, $Kf^*(G_n)$ and $Kf^+(G_n)$ are random variables.

Recall that G_{n+1} is G_n connected by an edge to a new terminal octagon H_{n+1}, where H_{n+1} is extended by vertices x_1, x_2, x_3, x_4, x_5, x_6, x_7, and x_8, and $p_n x_1$ is the new edge; see Figure 2. On the one hand, for all $m \in V_{G_n}$,

$$r(x_1, m) = r(p_n, m) + 1,\ r(x_2, m) = r(p_n, m) + 1 + \frac{7}{8},\ r(x_3, m) = r(p_n, m) + 1 + \frac{12}{8},\ r(x_4, m) = r(p_n, m) + 1 + \frac{15}{8}, \quad (17)$$

$$r(x_5, m) = r(p_n, m) + 1 + \frac{16}{8}, r(x_6, m) = r(p_n, m) + 1 + \frac{15}{8}, r(x_7, m) = r(p_n, m) + 1 + \frac{12}{8}, r(x_8, m) = r(p_n, m) + 1 + \frac{7}{8}. \quad (18)$$

$$\sum_{m \in V_{G_n}} d_{G_{n+1}}(m) = 18n - 1. \quad (19)$$

On the other hand, for all $t \in \{1, 2, 3, 4, 5, 6, 7, 8\}$

$$\sum_{t=1}^{8} d(x_t)r(x_1, x_t) = 21,\ \sum_{t=1}^{8} d(x_t)r(x_2, x_t) = \frac{175}{8},\ \sum_{t=1}^{8} d(x_t)r(x_3, x_t) = \frac{45}{2},\ \sum_{t=1}^{8} d(x_t)r(x_4, x_t) = \frac{183}{8}, \quad (20)$$

$$\sum_{t=1}^{8} d(x_t)r(x_5, x_t) = 23,\ \sum_{t=1}^{8} d(x_t)r(x_6, x_t) = \frac{183}{8},\ \sum_{t=1}^{8} d(x_t)r(x_7, x_t) = \frac{45}{2},\ \sum_{t=1}^{8} d(x_t)r(x_8, x_t) = \frac{175}{8}. \quad (21)$$

By Theorem 3.1 of [41], we have

$$E(Kf^*(G_n)) = (162 - \frac{243}{4}p_1 - 27p_2 - \frac{27}{4}p_3)n^3 + (36 + \frac{729}{4}p_1 + 81p_2 + \frac{81}{4}p_3)n^2 - (29 + \frac{243}{2}p_1 + 54p_2 + \frac{27}{2}p_3)n - 1.$$

we now present the first main result of this section.

Theorem 3. *The results are as follows, if Hypothesis 1 holds. As to the random cyclooctatetraene chain G_n, the variance of the multiplicative degree-Kirchhoff index $Kf^*(G_n)$, computed as*

$$Var(Kf^*(G_n)) = \frac{1}{30}(\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 + (-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)).$$

where

$$\sigma^2 = (\frac{1215}{2})^2 p_1 + 810^2 p_2 + (\frac{1863}{2})^2 p_3 + 972^2 p_4 - (\frac{1215}{2}p_1 + 810p_2 + \frac{1863}{2}p_3 + 972p_4)^2$$
$$\tilde{\sigma}^2 = (\frac{495}{2})^2 p_1 + 450^2 p_2 + (\frac{1143}{2})^2 p_3 + 612^2 p_4 - (\frac{495}{2}p_1 + 450p_2 + \frac{1143}{2}p_3 + 612p_4)^2$$
$$r = \frac{1215}{2} \cdot \frac{495}{2} \cdot p_1 + 810 \cdot 450 \cdot p_2 + \frac{1863}{2} \cdot \frac{1143}{2} \cdot p_3 + 972 \cdot 612 \cdot p_4 - (\frac{1215}{2}p_1 + 810p_2 + \frac{1863}{2}p_3 + 972p_4) \cdot (\frac{495}{2}p_1 + 450p_2 + \frac{1143}{2}p_3 + 612p_4)$$

Proof. By [41] (5.3), we have

$$Kf^*(G_{n+1}) = Kf^*(G_n) + 18 \sum_{m \in V_{G_n}} d(m) r(p_n, m) + 684n + 151. \tag{22}$$

and

$$C_n := 18 \sum_{m \in V_{G_n}} d(m) r(p_n, m). \tag{23}$$

$$Kf^*(G_{n+1}) = Kf^*(G_n) + C_n + 684n + 151. \tag{24}$$

□

Recalling from Section 1 that Z_n^1, Z_n^2, Z_n^3, and Z_n^4 are random variables, this indicates our option in constructing G_{n+1} from G_n. We have four equalities as follows:
Equality 1.

$$C_n Z_n^1 = (C_{n-1} + \frac{1215}{2}n - \frac{495}{2})Z_n^1$$

If $Z_n^1 = 0$, the above equality is obvious, so we only need to consider the case $Z_n^1 = 1$, which implies $G_n \longrightarrow G_{n+1}^1$. In this view, p_n (of G_n) is coincident with the vertex labeled x_2 or x_8 (of H_n), see Figure 4. In this scenario, C_n turns into

$$\begin{aligned}
C_n &= 18 \sum_{m \in V_{G_n}} d(m) r(x_2, m) \\
&= 18 \sum_{m \in V_{G_{n-1}}} d(m) r(x_2, m) + 18 \sum_{m \in V_{H_n}} d(m) r(x_2, m) \\
&= 18 \sum_{m \in V_{G_{n-1}}} d(m)(1 + \frac{7}{8} + r(p_{n-1}, m)) + \frac{175}{8} \times 18 \\
&= 18 \sum_{m \in V_{G_{n-1}}} d(m) r(p_{n-1}, m) + \frac{270}{8} \sum_{m \in V_{G_{n-1}}} d(m) + \frac{175}{8} \times 18 \\
&= C_{n-1} + \frac{270}{8}(18n - 19) + \frac{3150}{8} \\
&= C_{n-1} + \frac{1215}{2} n - \frac{495}{2}
\end{aligned}$$

In the foregoing, we utilised (17)–(19). As a result, we arrive at the required equivalence conclusion.

Equality 2.

$$C_n Z_n^2 = (C_{n-1} + 810n - 450) Z_n^2$$

As in the proof of Equality 1, we only have to regard the case $Z_n^2 = 1$, which is $G_n \longrightarrow G_{n+1}^2$. The proof process is analogous, and we leave out the details.

Equality 3.

$$C_n Z_n^3 = (C_{n-1} + \frac{1863}{2} n - \frac{1143}{2}) Z_n^3$$

We have to regard the case $Z_n^3 = 1$, which is $G_n \longrightarrow G_{n+1}^3$. The proof is the same as Equality 1 and we omit the details.

Equality 4.

$$C_n Z_n^4 = (C_{n-1} + 972n - 612) Z_n^4$$

We have to regard the case $Z_n^4 = 1$, which is $G_n \longrightarrow G_{n+1}^4$. The proof process is also analogous, and we leave out the details.

Recalling that $Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4 = 1$, according to the above discussion, it holds that

$$\begin{aligned}
C_n &= C_n(Z_n^1 + Z_n^2 + Z_n^3 + Z_n^4) \\
&= C_{n-1} + n \cdot U_n - V_n
\end{aligned}$$

where for each n, $U_n = \frac{1215}{2} Z_n^1 + 810 Z_n^2 + \frac{1863}{2} Z_n^3 + 972 Z_n^4$, $V_n = \frac{495}{2} Z_n^1 + 450 Z_n^2 + \frac{1143}{2} Z_n^3 + 612 Z_n^4$.

Therefore, by (22)

$$
\begin{aligned}
Kf^*(G_n) &= Kf^*(G_1) + \sum_{t=1}^{n-1} C_t + \sum_{t=1}^{n-1}(684t+151) \\
&= Kf^*(G_1) + \sum_{t=1}^{n-1}\Big(\sum_{q=1}^{t-1}(C_{q+1}-C_q) + C_1\Big) + \sum_{t=1}^{n-1}(684t+151) \\
&= Kf^*(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}(C_{q+1}-C_q) + (n-1)C_1 + \sum_{t=1}^{n-1}(684t+151) \\
&= Kf^*(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}((q+1)U_{q+1}-V_{q+1}) + (n-1)C_1 + \sum_{t=1}^{n-1}(684t+151) \\
&= Kf^*(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}((q+1)U_{q+1}-V_{q+1}) + O(n^2)
\end{aligned}
$$

Now, we consider $Kf^+(G_n)$. By Theorem 3.3 of [41] we have

$$
\begin{aligned}
E(Kf^+(G_n)) =&(144-54p_1-24p_2-6p_3)n^3 + (61+162p_1+72p_2+18p_3)n^2 \\
&-(37+108p_1+48p_2+12p_3)n.
\end{aligned}
$$

$Var(Kf^+(G_n))$ is given by

Theorem 4.

$$
\begin{aligned}
Var(Kf^+(G_n)) =&\frac{1}{30}(\sigma^2 n^5 - 5rn^4 + 10\tilde{\sigma}^2 n^3 + (65r - 30\sigma^2 - 45\tilde{\sigma}^2)n^2 \\
&+(-120r + 59\sigma^2 + 65\tilde{\sigma}^2)n + (60r - 30\sigma^2 - 30\tilde{\sigma}^2)).
\end{aligned}
$$

where

$$
\begin{aligned}
\sigma^2 =&540^2p_1 + 720^2p_2 + 828^2p_3 + 864^2p_4 - (540p_1 + 720p_2 + 828p_3 + 864p_4)^2 \\
\tilde{\sigma}^2 =&191^2p_1 + 371^2p_2 + 479^2p_3 + 515^2p_4 - (191p_1 + 371p_2 + 479p_3 + 515p_4)^2 \\
r =&540\cdot 191\cdot p_1 + 720\cdot 371\cdot p_2 + 828\cdot 479\cdot p_3 + 864\cdot 515\cdot p_4 \\
&-(540p_1 + 720p_2 + 828p_3 + 864p_4)\cdot(191p_1 + 371p_2 + 479p_3 + 515p_4)
\end{aligned}
$$

Proof. By [41] (5.4), we see that

$$
Kf^+(G_{n+1}) = Kf^+(G_n) + 18\sum_{m\in V_{G_n}} r(p_n,m) + 8\sum_{m\in V_{G_n}} d(m)r(p_n,m) + 637n + 160. \quad (25)
$$

where

$$
D_n := \sum_{m\in V_{G_n}} (18+8d(m))r(p_n,m). \quad (26)
$$

$$
Kf^+(G_{n+1}) = Kf^+(G_n) + D_n + 637n + 160. \quad (27)
$$

□

Recalling from Section 1 that Z_n^1, Z_n^2, Z_n^3, and Z_n^4 are random variables, this indicates our option in constructing G_{n+1} from G_n. We have four equalities as follows:
Equality 1.

$$
D_n Z_n^1 = (D_{n-1} + 540n - 191)Z_n^1
$$

If $Z_n^1 = 0$, the equality mentioned above is evident, so we only have to regard the case $Z_n^1 = 1$, which means that $G_n \longrightarrow G_{n+1}^1$. In this view, p_n (of G_n) is coincident with the vertex labeled x_2 or x_8 (of H_n), see Figure 4. In this scenario, D_n turns into

$$\begin{aligned}
\sum_{m\in V_{G_n}}(18+8d(m))r(x_2,m) &= 18\sum_{m\in V_{G_n}} d(m)r(x_2,m)\\
&= \sum_{m\in V_{G_{n-1}}}(18+8d(m))r(x_2,m)+\sum_{m\in V_{H_n}}(18+8d(m))r(x_2,m)\\
&= \sum_{m\in V_{G_{n-1}}}(18+8d(m))(r(p_{n-1},m)+1+\frac{7}{8})+18\sum_{m\in V_{H_n}} r(x_2,x_i)+8\sum_{m\in V_{H_n}} d(x_i)r(x_2,x_i)\\
&= \sum_{m\in V_{G_{n-1}}}(18+8d(m))r(p_{n-1},m)+\frac{15}{8}\sum_{m\in V_{G_{n-1}}}(18+8d(m))+364\\
&= D_{n-1}+\frac{15}{8}(288n-296)+364\\
&= D_{n-1}+540n-191
\end{aligned}$$

In the foregoing, we utilised (17)–(19). As a result, we arrive at the required equivalence conclusion.

Equality 2.

$$D_nZ_n^2 = (D_{n-1}+720n-371)Z_n^2$$

As in the proof of Equality 1, we only have to regard the case $Z_n^2 = 1$, which is $G_n \longrightarrow G_{n+1}^2$. The proof process is analogous, and we leave out the details.

Equality 3.

$$D_nZ_n^3 = (D_{n-1}+828n-479)Z_n^3$$

We have to regard the case $Z_n^3 = 1$, which is $G_n \longrightarrow G_{n+1}^3$. The proof is the same as Equality 1 and we omit the details.

Equality 4.

$$D_nZ_n^4 = (D_{n-1}+864n-515)Z_n^4$$

We have to regard the case $Z_n^4 = 1$, which is $G_n \longrightarrow G_{n+1}^4$. The proof process is also analogous, and we leave out the details.

Recalling that $Z_n^1+Z_n^2+Z_n^3+Z_n^4 = 1$, according to the above discussion, it holds that

$$\begin{aligned}
D_n &= D_n(Z_n^1+Z_n^2+Z_n^3+Z_n^4)\\
&= D_{n-1}+n\cdot U_n-V_n
\end{aligned}$$

where for each n, $U_n = 540Z_n^1+720Z_n^2+828Z_n^3+864Z_n^4$, $V_n = 191Z_n^1+371Z_n^2+479Z_n^3+515Z_n^4$.

Therefore, by (25)

$$
\begin{aligned}
Kf^{+}(G_n) &= Kf^{+}(G_1) + \sum_{t=1}^{n-1} D_t + \sum_{t=1}^{n-1}(637t+160) \\
&= Kf^{+}(G_1) + \sum_{t=1}^{n-1}\Big(\sum_{q=1}^{t-1}(D_{q+1}-D_q) + D_1\Big) + \sum_{t=1}^{n-1}(637t+160) \\
&= Kf^{+}(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}(D_{q+1}-D_q) + (n-1)D_1 + \sum_{t=1}^{n-1}(637t+160) \\
&= Kf^{+}(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}((q+1)U_{q+1}-V_{q+1}) + (n-1)D_1 + \sum_{t=1}^{n-1}(637t+160) \\
&= Kf^{+}(G_1) + \sum_{t=1}^{n-1}\sum_{q=1}^{t-1}((q+1)U_{q+1}-V_{q+1}) + O(n^2)
\end{aligned}
$$

If we replace $Gut(G_n)$ with $Kf^{+}(G_n)$ in the proof of Theorem 1, the rest of the proof of this theorem is the same as that in the proof of Theorem 1; we thus omit the details.

4. Concluding Remarks

In this paper, we obtain explicit analytical expressions for the variances of Schultz index, multiplicative degree-Kirchhoff index, Gutman index and additive degree-Kirchhoff index of a random cyclooctatetraene chain with n octagons. All of these results will contribute to the study of Schultz index, multiplicative degree-Kirchhoff index, Gutman index and additive degree-Kirchhoff index of graphs. With the continuous development and progress of science, more and more molecules are being discovered and created.

The polygonal chain problem in chemical graph theory has been extensively studied and discussed by researchers. For the variance of some certain indices of a random polygon chain that has n regular polygons, it is feasible to establish exact formulas.

Not only that, through these studies, we can hopefully obtain the variance of the n sided chain graph and some of their physicochemical properties in the near future.

Author Contributions: Conceptualization, C.T., S.T. and X.G.; methodology, C.T.; software, C.T.; validation, C.T. and X.G.; formal analysis, C.T.; investigation, C.T.; resources, S.T.; data curation, C.T.; writing—original draft preparation, C.T.; writing—review and editing, C.T.; visualization, S.T.; supervision, C.T.; project administration, C.T.; funding acquisition, X.G. All authors have read and agreed to the published version of the manuscript.

Funding: The research is partially supported by National Science Foundation of China (Grant No. 12171190) and Natural Science Foundation of Anhui Province (Grant No. 2008085MA01).

Data Availability Statement: Not applicable.

Acknowledgments: The authors are very grateful to the helpful comments and suggestions. The research is partially supported by National Science Foundation of China (Grant No. 12171190) and Natural Science Foundation of Anhui Province (Grant No. 2008085MA01).

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Bondy, J.A.; Murty, U.S.R. *Graph Theory*; Springer: New York, NY, USA, 2008.
2. Haruo, H.; Index, T. A Newly Proposed Quantity Characterizing the Topological Nature of Structural Isomers of Saturated Hydrocarbons. *J. Bull. Chem. Soc. Jpn.* **2006**, *44*, 2332–2339.
3. Estrada, E. Edge Adjacency Relationships and a Novel Topological Index Related to Molecular Volume. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 31–33. [CrossRef]
4. Person, W.B.; Pimentel, G.C.; Pitzer, K.S. The Structure of Cyclooctatetraene. *J. Am. Chem. Soc.* **1952**, *74*, 3437–3438. [CrossRef]
5. Cope, A.C.; Pike, R.M.; Polyolefins, C. Cyclooctatetraene Derivatives from Copolymerization and Side Chain Modification. *J. Am. Chem. Soc.* **1953**, *75*, 3220–3223. [CrossRef]

6. Luthe, G.; Jacobus, J.A.; Robertson, L.W. Receptor interactions by polybrominated diphenyl ethers versus polychlorinated biphenyls: A theoretical structure-activity assessment. *Environ. Toxicol. Pharm.* **2008**, *25*, 202–210. [CrossRef] [PubMed]
7. Mathews, F.S.; Lipscomb, W.N. The Structure of Silver Cyclooctatetraene Nitrate. *J. Phys. Chem.* **1959**, *63*, 845–850. [CrossRef]
8. Garavelli, M.; Bernardi, F.; Cembran, A. Cyclooctatetraene Computational Photo- and Thermal Chemistry: A Reactivity Model for Conjugated Hydrocarbons. *J. Am. Chem. Soc.* **2002**, *124*, 13770–13789. [CrossRef]
9. Lo, D.H.; Whitehead, M.A. Molecular geometry and bond energy. III. Cyclooctatetraene and related compounds. *J. Am. Chem. Soc.* **1969**, *91*, 238–242. [CrossRef]
10. Schwamm, R.J.; Anker, M.D.; Lein, M. Reduction vs. Addition: The Reaction of an Aluminyl Anion with 1,3,5,7-Cyclooctatetraene. *J. Chem.* **2019**, *58*, 1489–1493.
11. Milas, N.; Nolan, J., Jr.; Otto, P.H.L. Notes-Ozonization of Cyclooctatetraene. *J. Org. Chem.* **1958**, *23*, 624–625. [CrossRef]
12. Wiener, H. Structrual determination of paraffin boiling points. *J. Am. Chem. Soc.* **1947**, *69*, 17–20. [CrossRef] [PubMed]
13. Buckley, F.; Harary, F. *Distance in Graphs*; Addison-Wesley: Reading, UK, 1989.
14. Chen, A.L.; Zhang, F.J. Wiener index and perfect matchings in random phenylene chains. *MATCH Commun. Math. Comput. Chem.* **2009**, *61*, 623–630.
15. Entringer, R.C.; Jackson, D.E.; Snyder, D.A. Distance in graphs. *Czechoslov. Math. J.* **1976**, *26*, 283–296. [CrossRef]
16. Zhou, Q.N.; Wang, L.G.; Lu, Y. Wiener index and Harary index on Hamilton-connected graphs with large minimum degree. *Discrete Appl. Math.* **2018**, *247*, 180–185. [CrossRef]
17. Zhang, L.I.; Li, Q.S.; Li, S.C.; Zhang, M.J. The expected values for the Schultz index, Gutman index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random polyphenylene chain. *J. Discret. Appl. Math.* **2020**, *282*, 243–256. [CrossRef]
18. Zhang, J.L.; Peng, X.H.; Chen, H.L. The limiting behaviours for the Gutman index, Schultz index,multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random polyphenylene chain. *Discrete Appl. Math.* **2021**, *299*, 62–73. [CrossRef]
19. Ayache, A.; Alameri, A. Topological indices of the m^k-graph. *J. Assoc. Arab. Univ. Basic Appl. Sci.* **2017**, *24*, 283–291.
20. Gutman, I. Selected properties of the Schultz molecular topological index. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 1087–1089. [CrossRef]
21. Chen, S. Modified Schultz index of zig-zag polyhex nanotubes. *J. Comput. Theor. Nanosci.* **2009**, *6*, 1499–1503. [CrossRef]
22. Farahani, M.R. Hosoya, Schultz, modified Schultz polynomials and their topological indices of benzene molecules: First members of polycyclic aromatic hydrocarbons (PAHs). *Int. J. Theor. Chem.* **2013**, *1*, 9–16.
23. Heydari, A. On the modified Schultz index of $C_4C_8(S)$ nanotubes and nanotorus. *Digest. J. Nanomater. Biostruct.* **2010**, *5*, 51–56.
24. Xiao, Z.; Chen, S. The modified Schultz index of armchair polyhex nanotubes. *J. Comput. Theor. Nanosci.* **2009**, *6*, 1109–1114. [CrossRef]
25. Mukwembi, S.; Munyira, S. MunyiraDegree distance and minimum degree. *Bull. Aust. Math. Soc.* **2013**, *87*, 255–271. [CrossRef]
26. Qi, X.L.; Zhou, B.; Du, Z.B. The Kirchhoff indices and the matching numbers of unicyclic graphs. *J. Appl. Math. Comput.* **2016**, *289*. [CrossRef]
27. Georgakopoulos, A. Uniqueness of electrical currents in a network of finite total resistance. *J. Lond. Math. Soc.* **2010**, *82*, 256–272. [CrossRef]
28. Huang, S.B.; Zhou, J.; Bu, C.J. Some results on Kirchhoff index and degree-Kirchhoff index. *MATCH Commun. Math. Comput. Chem.* **2016**, *75*, 207–222.
29. Cinkir, Z. Deletion and contraction identities for the resistance calues and the Kirchhoff index. *Int. J. Quantum Chem.* **2011**, *111*, 4030–4041. [CrossRef]
30. Gupta, S.; Singh, M.; Madan, A.K. Eccentric distance sum: A novel graph invariant for predicting biological and physical properties. *J. Math. Anal. Appl.* **2002**, *275*, 386–401. [CrossRef]
31. Klein, D.J.; Randić, M. Resistance distance. *J. Math. Chem.* **1993**, *12*, 81–95. [CrossRef]
32. He, F.G.; Zhu, Z.X. Cacti with maximum eccentricity resistance-distance sum. *Discret. Appl. Math.* **2017**, *219*, 117–125. [CrossRef]
33. Huang, Z.W.; Xi, X.Z.; Yuan, S.L. Some further results on the eccentric distance sum. *J. Math. Anal. Appl.* **2019**, *470*, 145–158. [CrossRef]
34. Li, S.C.; Wei, W. Some edge-grafting transformations on the eccentricity resistance-distance sum and their applications. *Discret. Appl. Math.* **2016**, *211*, 130–142. [CrossRef]
35. Somodi, M. On the Ihara zeta function and resistance distance-based indices. *Linear Algebra Appl.* **2017**, *513*, 201–209. [CrossRef]
36. Yang, Y.J.; Klein, D.J. A note on the Kirchhoff and additive degree-Kirchhoff indices of graphs. *Z. Naturforsch. A* **2015**, *70*, 459–463. [CrossRef]
37. Chen, H.; Zhang, F. Resistance distance and the normalized Laplacian spectrum. *Discret. Appl. Math.* **2007**, *155*, 654–661. [CrossRef]
38. Tang, M.; Priebe, C.E. Limit theorems for eigenvectors of the normalized Laplacian for random graphs. *Ann. Statist.* **2018**, *46*, 2360–2415. [CrossRef]
39. Chung, F.R.K. *Spectral Graph Theory*; American Mathematical Society: Providence, RI, USA, 1997.

40. Gutman, I.; Feng, L.; Yu, G. Degree resistance distance of unicyclic graphs. *Trans. Comb.* **2012**, *1*, 27–40.
41. Qi, J.F.; Ni, J.B.; Geng, X.Y. The expected values for the Kirchhoff indices in the random cyclooctatetraene and spiro chains. *J. Discret. Appl. Math.* **2022**, *321*, 240–249. [CrossRef]