The expected values for the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random cyclooctatetraene chain*

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Abstract: In this paper, we mainly solve the explicit analytical expressions for the expected values of the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random cyclooctatetraene chain with n octagons. We also obtain the average values of these four indices with respect to the set of all these cyclooctatetraene chains.

Keywords: Random cyclooctatetraene chain; Gutman index; Schultz index; Multiplicative degree-Kirchhoff index; Additive degree-Kirchhoff index

1. Introduction

In this paper, we only consider simple and finite connected graphs, we refer to [2] and the references cited therein. Chemistry has been widely studied and applied in graph theory. The chemical compounds can be described in chemical graph theory, vertices represent the atoms and edges stand for the covalent bonds between atoms.

Predicting the physicochemical properties of compounds is considered to be an attractive problem in theoretical chemistry. Many predictive methods are being and have been developed to connect molecular structures and their physicochemical properties. One of the most important methods in chemical graph theory are usually called topological indices. According to the different parameters such as point degree, adjacent point degree and distance between two points, topological indices can be divided into many categories.

Hydrocarbons are a kind of very important substances, and their derivatives has always been an important research topic in the field of organic chemistry. Cyclooctatetraene is a typical unsaturated hydrocarbon, so more and more people study its structure and properties, and the research in chemical graph theory is more and more in-depth. In this article, we consider four kinds indices of cyclooctatetraene chains with n octagons. For more information, we can refer to [11, 27, 30, 34].

Let $G = (V_G, E_G)$ be a graph with vertex set V_G and the edge set E_G. The distance, $d_G(u, v)$ (or $d(u, v)$ for short), between vertices u and v of G is the length of a shortest $u, v - path$ in G. The famous Wiener index (or transmission) $\omega(G)$ of E_G is the sum of distances between all pairs of vertices of G. It was created by Harry Wiener in 1947 [37], that is,

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

The Wiener index is calculated in several survey papers (see [4, 9, 22, 38]) and is more and more widely used and studied, see [21, 26, 45].

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A weighted graph [44] (G,ω) is a graph $G=(V_G,E_G)$ together with the weight function ω: $V_G\to\mathbb{N}^+$. Let $\oplus$ denote one of the four operations $+,-,\times,\div$. The weighted Wiener index $W(G,\omega)$ is defined as

$$W(G,\omega)=\frac{1}{2}\sum_{u\in V_G}\sum_{v\in V_G}(\omega(u)\oplus\omega(v))d_G(u,v). \tag{1.1}$$

Clearly, if $\omega\equiv 1$ and $\oplus$ denotes the operation $\times$, then $W(G,\omega)=W(G)$.

If $\oplus$ denotes the operation $\times$ and $\omega(\cdot)\equiv d_G(\cdot)$, the corresponding vertex degree, then (1.1) is equivalent to

$$Gut(G)=\frac{1}{2}\sum_{u\in V_G}\sum_{v\in V_G}(d_G(u)d_G(v))d_G(u,v)=\sum_{\{u.v\}\subseteq V_G}(d_G(u)d_G(v))d_G(u,v), \tag{1.2}$$

which is just the Gutman index. For the study of the possible chemical applications of Gutman index, and similar quantities, as well as their theoretical studies, polycyclic molecules are more difficult cases, see [3, 39].

If $\oplus$ denotes the operation $+$ and $\omega(\cdot)\equiv d_G(\cdot)$, then (1.1) is equivalent to

$$S(G)=\frac{1}{2}\sum_{u\in V_G}\sum_{v\in V_G}(d_G(u)+d_G(v))d_G(u,v)=\sum_{\{u.v\}\subseteq V_G}(d_G(u)+d_G(v))d_G(u,v), \tag{1.3}$$

which is just the Schultz index. More articles on developing such a topology indexes of the [10, 16].

The resistance distance $r(x,y)$ is the potential difference between x and y of G induced by the unique $x-y$ flow intensity 1 satisfying Kirchhoffs cycle law [12], for more detailed information in [7, 13, 18]. The Wiener index for non-trees is the Kirchhoff index, this distance funtion proposed by Klein and Randić [20], defined as

$$Kf(G)=\sum_{\{x,y\}\subseteq V_G}r(x,y),$$

there are introduced the eccentric distance sum and the eccentricity resistance-distance sum, refer to [15, 19, 24].

In 2007, The multiplicative degree-Kirchhoff index was proposed by Chen and Zhang in [5], which was defined as

$$Kf^*(G)=\sum_{\{x,y\}\subseteq V_G}d(x)d(y)r(x,y)=2|E_G|\sum_{i=2}^{n}\frac{1}{\lambda_i}, \tag{1.4}$$

where $0=\lambda_1<\lambda_2\leq\cdots\leq\lambda_n$ are the eigenvalues of $\ell(G)$. Here, $\ell(G)$ is the normalized Laplacian matrix of the graph G, which was proposed by Chung [6]. The normalized Laplacian index and multiplicative degree-Kirchhoff index have important applications in mathematical chemistry and statistics. Their research has attracted more and more researchers' attention, which can be seen in [1, 25, 31].

In 2012, Gutman, Feng and Yu [14] introduced the additive degree-Kirchhoff index, which was defined as

$$Kf^+(G)=\sum_{\{x,y\}\subseteq V_G}(d(x)+d(y))r(x,y). \tag{1.5}$$

For the results on the additive degree-Kirchhoff index, one may be referred to Refs.[32, 41, 42].

A random cyclooctatetraene chain G_n with n octagons can be considered as a cyclooctatetraene chain G_{n-1} with $n-1$ octagons to which a new terminal octagon H_n has been adjoined by a cut edge, see Figure1. For $n\geq 3$, the terminal octagon H_n can be attached in four ways, which results in the local arrangements we describe as G_n^1, G_n^2, G_n^3, G_n^4, see Figure 2. A random cyclooctatetraene chain $G_n(p_1,\ p_2,\ p_3)$ with n octagons is a cyclooctatetraene chain obtained by stepwise addition of terminal octagons. At each step $k(=3,4,\ldots,n)$ a random selection is made from one of the four possible constructions:

- $G_{k-1}\to G_k^1$ with probability p_1,
- $G_{k-1}\to G_k^2$ with probability p_2,
- $G_{k-1}\to G_k^3$ with probability p_3,
- $G_{k-1}\to G_k^4$ with probability $p_4=1-p_1-p_2-p_3$,

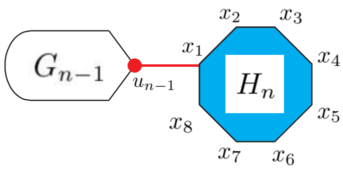

Figure 1: A cyclooctatetraene chain G_n with n octagons.

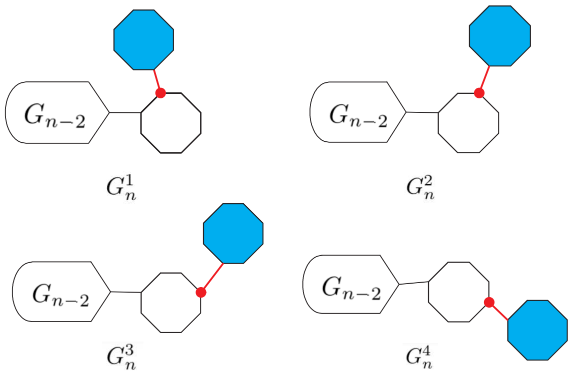

Figure 2: The four types of local arrangements in cyclooctatetraene chains.

where the probabilities p_1, p_2 and p_3 are constants, irrelative to the step parameter k.

Let G_n be a cyclooctatetraene chain with n octagons $H_1, H_2, \ldots, H_n$. Set $u_k\omega_k$ be the cut edge of G_n connecting H_k and H_{k+1} with $u_k \in V_{H_k}$, $\omega_k \in V_{H_{k+1}}$ for $k = 1, 2, \ldots, n-1$. Clearly, both ω_k and u_{k+1} are the vertices in H_{k+1} and $d(\omega_k, u_{k+1}) \in \{1, 2, 3, 4\}$. Specially, G_n is the meta-chain M_n, the ortho-chain O_n^1, O_n^2 and the para-chain L_n if $d(\omega_k, u_{k+1}) = 1$ (*i.e.*, $p_1 = 1$), $d(\omega_k, u_{k+1}) = 2$ (*i.e.*, $p_2 = 1$), $d(\omega_k, u_{k+1}) = 3$ (*i.e.*, $p_3 = 1$) and $d(\omega_k, u_{k+1}) = 4$ (*i.e.*, $p_4 = 1$) for all $k \in \{1, 2, \ldots, n-2\}$, respectively.

Yang and Zhang [40] and Ma et al. [29], independently, obtained a simple exact formula for the expected value of the Wiener index of a random polyphenylene chain. Huang, Kuang and Deng [17] obtained the expected values of the Kirchhoff index of random polyphenyl and spiro chains. Wei and Shiu [36] gave the simple formulas of the expected value of the Wiener index of random polygonal chain. Very recently, Zhang, Li, Li and one of the authors of this paper obtained the expected values of the expected values for the Schultz index, Gutman index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random polyphenylene chain, see in [44]. Zhang, Peng and Chen [43] established the explicit analytical expressions for the variance of the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degreeKirchhoff index of a random polyphenylene chain. In [23], the explicit analytical expressions for the expected values of the Kirchhoff index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index in random polygonal chains were established by solving a difference equation.

Motivated by these results, in this paper, we calculate the explicit analytical expressions for the expected values of the Gutman index, the Schultz index, the multiplicative degree-Kirchhoff index and the additive degree-Kirchhoff index of a random cyclooctatetraene chain. We also obtain the average values of these four indices with respect to the set of all cyclooctatetraene chains with n octagons. The following are our main results:

Theorem 1.1. *For $n \geq 1$, the expected value of the Gutman index, the Schultz index, the multiplicative degree-Kirchhoff index and the additive degree-Kirchhoff indexof random cyclooctatetraene chain G_n, respectively, are*

$$\begin{aligned} E(Gut(G_n)) &= (270 - 162p_1 - 108p_2 - 54p_3)n^3 + (486p_1 + 324p_2 + 162p_3 - 90)n^2 \\ &\quad +(77 - 324p_1 - 216p_2 - 108p_3)n - 1; \qquad (1.6) \\ E(S(G_n)) &= (240 - 144p_1 - 96p_2 - 48p_3)n^3 + (432p_1 + 288p_2 + 144p_3 - 40)n^2 \\ &\quad +(56 - 288p_1 - 192p_2 - 96p_3)n; \qquad (1.7) \end{aligned}$$

$$E(Kf^*(G_n)) = (162 - \frac{243}{4}p_1 - 27p_2 - \frac{27}{4}p_3)n^3 + (36 + \frac{729}{4}p_1 + 81p_2 + \frac{81}{4}p_3)n^2 - (29 + \frac{243}{2}p_1 + 54p_2 + \frac{27}{2}p_3)n - 1; \quad (1.8)$$

$$E(Kf^*(G_n)) = (-\frac{243}{4}n^3 + \frac{729}{4}n^2 - \frac{243}{2}n)(1 - p_2) + (-27n^3 + 81n^2 - 54n)p_2 + 162n^3 + 36n^2 - 29n - 1. \quad (1.9)$$

Corollary 1.2. *For a random cyclooctatetraene chain G_n ($n \geq 3$), the para-chain L_n realizes the maximum of $E(Gut(G_n)), E(S(G_n)), E(Kf^*(G_n))$ and $E(Kf^*(G_n))$, respectively, while the meta-chain M_n realizes these of minimum.*

For convenience, let Θ_n be the set of all cyclooctatetraene chains with n octagons. We give the average values of the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index with respect to Θ_n.

$$Gut_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{G\in\Theta_n} Gut(G), \qquad S_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{G\in\Theta_n} S(G),$$

$$Kf^*_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{G\in\Theta_n} Kf^*(G), \quad Kf^+_{avr}(\Theta_n) = \frac{1}{|\Theta_n|}\sum_{G\in\Theta_n} Kf^+(G).$$

For achieving the average value $Gut_{avr}(\Theta_n)$ (resp. $S_{avr}(\Theta_n)$, $Kf^*_{avr}(\Theta_n)$, $Kf^+_{avr}(\Theta_n)$), It takes $p_1 = p_2 = p_3 = p_4 = \frac{1}{4}$ in the expected value $E(Gut(G_n))$ (resp. $E(S(G_n))$, $E(Kf^*(G_n))$, $E(Kf^+(G_n))$). According to Theorem 1.1, we have

Theorem 1.3. *For $n \geq 1$, the average values of the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index with respect to Θ_n are*

$$Gut_{avr}(\Theta_n) = 189n^3 + 153n^2 - 85n - 1, \qquad S_{avr}(\Theta_n) = 168n^3 + 176n^2 - 88n,$$

$$Kf^*_{avr}(\Theta_n) = \frac{1107}{8}n^3 + \frac{855}{8}n^2 - \frac{305}{4}n - 1, \quad Kf^+_{avr}(\Theta_n) = 123n^3 + 124n^2 - 79n.$$

After validation, the following equations are established,

$$Gut_{avr}(\Theta_n) = \frac{1}{4}Gut(M_n) + \frac{1}{4}Gut(O_n^1) + \frac{1}{4}Gut(O_n^2) + \frac{1}{4}Gut(L_n),$$

$$S_{avr}(\Theta_n) = \frac{1}{4}S(M_n) + \frac{1}{4}S(O_n^1) + \frac{1}{4}S(O_n^2) + \frac{1}{4}S(L_n),$$

$$Kf^*_{avr}(\Theta_n) = \frac{1}{4}Kf^*(M_n) + \frac{1}{4}Kf^*(O_n^1) + \frac{1}{4}Kf^*(O_n^2) + \frac{1}{4}Kf^*(L_n),$$

$$Kf^+_{avr}(\Theta_n) = \frac{1}{4}Kf^+(M_n) + \frac{1}{4}Kf^+(O_n^1) + \frac{1}{4}Kf^+(O_n^2) + \frac{1}{4}Kf^+(L_n).$$

2. Proofs of (1.6) and (1.7) in Theorem 1.1

In this section, we give the proofs of (1.6) and (1.7) in Theorem 1.1. Note that G_{n+1} is obtained from G_n by attaching a new terminal octagon H_{n+1} through an edge, where H_{n+1} is spanned by vertices x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, and the new edge is u_nx_1; see Figure 1.

Consider the distance between a vertex in V_{G_n} and a vertex in $V_{H_{n+1}}$, for any $v \in V_{G_n}$, one has

$$d(x_1, v) = d(u_n, v) + 1, \quad d(x_2, v) = d(u_n, v) + 2, \quad d(x_3, v) = d(u_n, v) + 3, \quad d(x_4, v) = d(u_n, v) + 4, \quad (2.1)$$

$$d(x_5, v) = d(u_n, v) + 5, \quad d(x_6, v) = d(u_n, v) + 4, \quad d(x_7, v) = d(u_n, v) + 3, \quad d(x_8, v) = d(u_n, v) + 2, \quad (2.2)$$

$$\sum_{v\in V_{G_n}} d_{G_{n+1}}(v) = 18n - 1. \quad (2.3)$$

Consider the distance between two vertices in $V_{H_{n+1}}$, one has

$$\sum_{i=1}^{8} d(x_i)d(x_1,x_i)=32,\quad \sum_{i=1}^{8} d(x_i)d(x_2,x_i)=33,\quad \sum_{i=1}^{8} d(x_i)d(x_3,x_i)=34,\quad \sum_{i=1}^{8} d(x_i)d(x_4,x_i)=35, \tag{2.4}$$

$$\sum_{i=1}^{8} d(x_i)d(x_5,x_i)=36,\quad \sum_{i=1}^{8} d(x_i)d(x_6,x_i)=35,\quad \sum_{i=1}^{8} d(x_i)d(x_7,x_i)=34,\quad \sum_{i=1}^{8} d(x_i)d(x_8,x_i)=33. \tag{2.5}$$

Firstly, we prove that (1.6) holds. By (1.2) one has

$$Gut(G_{n+1}) = \sum_{\{u,v\}\subseteq V_{G_n}} d(u)d(v)d(u,v) + \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} d(v)d(x_i)d(v,x_i) + \sum_{\{x_i,x_j\}\subseteq V_{H_{n+1}}} d(x_i)d(x_j)d(x_i,x_j).$$

Note that

$$\begin{aligned}
\sum_{\{u,v\}\subseteq V_{G_n}} d(u)d(v)d(u,v) &= \sum_{\{u,v\}\subseteq V_{G_n}\setminus\{u_n\}} d(u)d(v)d(u,v) + \sum_{v\in V_{G_n}\setminus\{u_n\}} d_{G_{n+1}}(u_n)d(v)d(u_n,v)\\
&= \sum_{\{u,v\}\subseteq V_{G_n}\setminus\{u_n\}} d(u)d(v)d(u,v) + \sum_{v\in V_{G_n}\setminus\{u_n\}} (d_{G_n}(u_n)+1)d(v)d(u_n,v)\\
&= Gut(G_n) + \sum_{v\in V_{G_n}} d(v)d(u_n,v).
\end{aligned}$$

Recall that $d(x_1)=3$ and $d(x_i)=2$ for $i\in\{2,3,4,5,6,7,8\}$. From (2.1)-(2.3), we have

$$\begin{aligned}
&\sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} d(v)d(x_i)d(v,x_i)\\
=&\sum_{v\in V_{G_n}} d(v)[3(d(u_n,v)+1)+2(d(u_n,v)+2)+2(d(u_n,v)+3)+2(d(u_n,v)+4)\\
&+2(d(u_n,v)+5)+2(d(u_n,v)+4)+2(d(u_n,v)+3)+2(d(u_n,v)+2)]\\
=&\sum_{v\in V_{G_n}} d(v)(17d(u_n,v)+49)\\
=&17\sum_{v\in V_{G_n}} d(v)d(u_n,v)+49\sum_{v\in V_{G_n}} d(v)\\
=&17\sum_{v\in V_{G_n}} d(v)d(u_n,v)+49(18n-1).
\end{aligned}$$

From (2.4)-(2.5), one has

$$\begin{aligned}
\sum_{\{x_i,x_j\}\subseteq V_{H_{n+1}}} d(x_i)d(x_j)d(x_i,x_j) =&\frac{1}{2}\sum_{i=1}^{8} d(x_i)(\sum_{j=1}^{8} d(x_j)d(x_i,x_j))\\
=&\frac{1}{2}[3\times 32+2\times 33+2\times 34+2\times 35+2\times 36+2\times 35+2\times 34+2\times 33]\\
=&288.
\end{aligned}$$

Thus,

$$Gut(G_{n+1}) = Gut(G_n) + 18\sum_{v\in V_{G_n}} d(v)d(u_n,v) + 882n + 239. \tag{2.6}$$

For a random cyclooctatetraene chain G_n, the number $\sum_{v\in V_{G_n}} d(v)d(u_n,v)$ is a random variable. We may denote its expected value by

$$A_n := E(\sum_{v\in V_{G_n}} d(v)d(u_n,v)).$$

By a direct calculation and (2.6), we can obtain a recurrence relation for the expected values of the Gutman index of a random cyclooctatetraene chain G_n as follows,

$$E(Gut(G_{n+1})) = E(Gut(G_n)) + 18A_n + 882n + 239.$$

Considering the following four possible cases.
Case1. $G_n \longrightarrow G^1_{n+1}$. In this case, $u_n(of G_n)$ considers the vertex x_2 or x_8. Consequently, $\sum_{v\in V_{G_n}} d(v)d(u_n, v)$ is given by $\sum_{v\in V_{G_n}} d(v)d(x_2, v)$ or $\sum_{v\in V_{G_n}} d(v)d(x_8, v)$ with probability p_1.
Case2. $G_n \longrightarrow G^2_{n+1}$. In this case, $u_n(of G_n)$ considers the vertex x_3 or x_7. Consequently, $\sum_{v\in V_{G_n}} d(v)d(u_n, v)$ is given by $\sum_{v\in V_{G_n}} d(v)d(x_3, v)$ or $\sum_{v\in V_{G_n}} d(v)d(x_7, v)$ with probability p_2.
Case3. $G_n \longrightarrow G^3_{n+1}$. In this case, $u_n(of G_n)$ considers the vertex x_4 or x_6. Consequently, $\sum_{v\in V_{G_n}} d(v)d(u_n, v)$ is given by $\sum_{v\in V_{G_n}} d(v)d(x_4, v)$ or $\sum_{v\in V_{G_n}} d(v)d(x_6, v)$ with probability p_3.
Case4. $G_n \longrightarrow G^4_{n+1}$. In this case, $u_n(of G_n)$ considers the vertex x_5. Consequently, $\sum_{v\in V_{G_n}} d(v)d(u_n, v)$ is given by $\sum_{v\in V_{G_n}} d(v)d(x_5, v)$ with probability $1 - p_1 - p_2 - p_3$.

According to the above four cases, we may obtain the expected value A_n as

$$\begin{aligned}
A_n =& p_1 \sum_{v\in V_{G_n}} d(v)d(x_2, v) + p_2 \sum_{v\in V_{G_n}} d(v)d(x_3, v) + p_3 \sum_{v\in V_{G_n}} d(v)d(x_4, v) + (1 - p_1 - p_2 - p_3) \sum_{v\in V_{G_n}} d(v)d(x_5, v) \\
=& p_1[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + 2 \sum_{v\in V_{G_{n-1}}} d(v) + 33] \\
&+ p_2[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + 3 \sum_{v\in V_{G_{n-1}}} d(v) + 34] \\
&+ p_3[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + 4 \sum_{v\in V_{G_{n-1}}} d(v) + 35] \\
&+ (1 - p_1 - p_2 - p_3)[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1}, v) + 5 \sum_{v\in V_{G_{n-1}}} d(v) + 36].
\end{aligned}$$

By applying the expected operator to the above equation, and noting that $E(A_n) = A_n$, we obtain

$$\begin{aligned}
A_n =& p_1(A_{n-1} + 36n - 5) + p_2(A_{n-1} + 54n - 23) + p_3(A_{n-1} + 72n - 41) + (1 - p_1 - p_2 - p_3)(A_{n-1} + 90n - 59) \\
=& A_{n-1} + (90 - 54p_1 - 36p_2 - 18p_3)n + 54p_1 + 36p_2 + 18p_3 - 59.
\end{aligned}$$

The boundary condition is

$$A_1 = E(\sum_{v\in V_{G_1}} d(v)d(u_1, v)) = 32.$$

According to the above recurrence relation and the boundary condition, we have

$$A_n = (45 - 27p_1 - 18p_2 - 9p_3)n^2 + (27p_1 + 18p_2 + 9p_3 - 14)n + 1.$$

Therefore,

$$\begin{aligned}
E(Gut(G_{n+1})) &= E(Gut(G_n)) + 18A_n + 882n + 239 \\
&= E(Gut(G_n)) + 18[(45 - 27p_1 - 18p_2 - 9p_3)n^2 + (27p_1 + 18p_2 + 9p_3 - 14)n + 1] + 882n + 239,
\end{aligned}$$

and the boundary condition is $E(Gut(G_1)) = 256$.

According to the above recurrence relation and the boundary condition, we have

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

(1.6) holds.

Then, we prove that (1.7) holds. By (1.3), one has

$$S(G_{n+1}) = \sum_{\{u,v\}\subseteq V_{G_n}} (d(u)+d(v))d(u,v) + \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} (d(v)+d(x_i))d(v,x_i)$$
$$+ \sum_{\{x_i,x_j\}\subseteq V_{H_{n+1}}} (d(x_i)+d(x_j))d(x_i,x_j).$$

By a similar discussion as the proof of (1.6), one has

$$\begin{aligned}\sum_{\{u,v\}\subseteq V_{G_n}} (d(u)+d(v))d(u,v) &= \sum_{\{u,v\}\subseteq V_{G_n}\setminus\{u_n\}} (d(u)+d(v))d(u,v) + \sum_{v\in V_{G_n}\setminus\{u_n\}} (d_{G_{n+1}}(u_n)+d(v))d(u_n,v)\\ &= \sum_{\{u,v\}\subseteq V_{G_n}\setminus\{u_n\}} (d(u)+d(v))d(u,v) + \sum_{v\in V_{G_n}\setminus\{u_n\}} (d_{G_n}(u_n)+1+d(v))d(u_n,v)\\ &= S(G_n) + \sum_{v\in V_{G_n}} d(u_n,v).\end{aligned}$$

Recall that $d(x_1)=3$ and $d(x_i)=2$ for $i\in\{2,3,4,5,6,7,8\}$. From (2.1)-(2.3), we have

$$\begin{aligned}&\sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} (d(v)+d(x_i))d(v,x_i)\\ =&\sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} d(v)d(v,x_i) + \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} d(x_i)d(v,x_i)\\ =&\sum_{v\in V_{G_n}} d(v)[(d(u_n,v)+1)+(d(u_n,v)+2)+(d(u_n,v)+3)+(d(u_n,v)+4)\\ &+(d(u_n,v)+5)+(d(u_n,v)+4)+(d(u_n,v)+3)+(d(u_n,v)+2)]\\ &+\sum_{v\in V_{G_n}} [3(d(u_n,v)+1)+2(d(u_n,v)+2)+2(d(u_n,v)+3)+2(d(u_n,v)+4)\\ &+2(d(u_n,v)+5)+2(d(u_n,v)+4)+2(d(u_n,v)+3)+2(d(u_n,v)+2)]\\ =&\sum_{v\in V_{G_n}} d(v)(8d(u_n,v)+24) + \sum_{v\in V_{G_n}} (17d(u_n,v)+49)\\ =&8\sum_{v\in V_{G_n}} d(v)d(u_n,v) + 24(18n-1) + 17\sum_{v\in V_{G_n}} d(u_n,v) + 49\times 8n.\end{aligned}$$

Note that $\sum_{i=1}^{8} d(x_k,x_i)=16$ for $k=1,2,3,4,5,6,7,8$. From (2.4)-(2.5), one has

$$\begin{aligned}\sum_{\{x_i,x_j\}\subseteq V_{H_{n+1}}} (d(x_i)+d(x_j))d(x_i,x_j) =&\frac{1}{2}\sum_{i=1}^{8}\sum_{j=1}^{8}(d(x_i)+d(x_j))d(x_i,x_j)\\ =&\sum_{i=1}^{8}\sum_{j=1}^{8} d(x_i)d(x_i,x_j) = 16\times(3+2\times 7)\\ =&272.\end{aligned}$$

Then

$$S(G_{n+1}) = S(G_n) + 18\sum_{v\in V_{G_n}} d(u_n,v) + 8\sum_{v\in V_{G_n}} d(v)d(u_n,v) + 824n + 248. \tag{2.7}$$

For a random cyclooctatetraene chain G_n, the number $\sum_{v\in V_{G_n}} d(u_n,v)$ is a random variable. We may denote its expected value by

$$B_n := E(\sum_{v\in V_{G_n}} d(u_n,v)).$$

By a direct calculation and (2.7), we can obtain a recurrence relation for the expected values of the Schuitz index of a random cyclooctatetraene chain G_n as follows,

$$E(S(G_{n+1})) = E(S(G_n)) + 18B_n + 8A_n + 824n + 248.$$

Considering the following four possible cases.

Case1. $G_n \longrightarrow G^1_{n+1}$. In this case, u_n is the vertex x_2 or x_8. Consequently, $\sum_{v\in V_{G_n}} d(u_n, v)$ is given by $\sum_{v\in V_{G_n}} d(x_2, v)$ or $\sum_{v\in V_{G_n}} d(x_8, v)$ with probability p_1.

Case2. $G_n \longrightarrow G^2_{n+1}$. In this case, u_n is the vertex x_3 or x_7. Consequently, $\sum_{v\in V_{G_n}} d(u_n, v)$ is given by $\sum_{v\in V_{G_n}} d(x_3, v)$ or $\sum_{v\in V_{G_n}} d(x_7, v)$ with probability p_2.

Case3. $G_n \longrightarrow G^3_{n+1}$. In this case, u_n is the vertex x_4 or x_6. Consequently, $\sum_{v\in V_{G_n}} d(u_n, v)$ is given by $\sum_{v\in V_{G_n}} d(x_4, v)$ or $\sum_{v\in V_{G_n}} d(x_6, v)$ with probability p_3.

Case4. $G_n \longrightarrow G^4_{n+1}$. In this case, u_n is the vertex x_5. Consequently, $\sum_{v\in V_{G_n}} d(u_n, v)$ is given by $\sum_{v\in V_{G_n}} d(x_5, v)$ with probability $1 - p_1 - p_2 - p_3$.

According to the above four cases, we may obtain the expected value B_n as

$$\begin{aligned}
B_n =& p_1 \sum_{v\in V_{G_n}} d(x_2, v) + p_2 \sum_{v\in V_{G_n}} d(x_3, v) + p_3 \sum_{v\in V_{G_n}} d(x_4, v) + (1 - p_1 - p_2 - p_3) \sum_{v\in V_{G_n}} d(x_5, v) \\
=& p_1[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + 2 \times 8(n - 1) + 16] \\
&+ p_2[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + 3 \times 8(n - 1) + 16] \\
&+ p_3[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + 4 \times 8(n - 1) + 16] \\
&+ (1 - p_1 - p_2 - p_3)[\sum_{v\in V_{G_{n-1}}} d(u_{n-1}, v) + 5 \times 8(n - 1) + 16].
\end{aligned}$$

By applying the expected operator to the above equation, and noting that $E(B_n) = B_n$, we obtain

$$\begin{aligned}
B_n =& p_1(B_{n-1} + 16n) + p_2(B_{n-1} + 24n - 8) + p_3(B_{n-1} + 32n - 16) + (1 - p_1 - p_2 - p_3)(B_{n-1} + 40n - 24) \\
=& B_{n-1} + (40 - 24p_1 - 16p_2 - 8p_3)n + 24p_1 + 16p_2 + 8p_3 - 24.
\end{aligned}$$

The boundary condition is

$$B_1 = E(\sum_{v\in V_{G_1}} d(u_1, v)) = 16.$$

According to the above recurrence relation and the boundary condition, we have

$$B_n = (20 - 12p_1 - 8p_2 - 4p_3)n^2 + (12p_1 + 8p_2 + 4p_3 - 4)n.$$

Recall that

$$A_n = (45 - 27p_1 - 18p_2 - 9p_3)n^2 + (27p_1 + 18p_2 + 9p_3 - 14)n + 1.$$

Therefore,

$$\begin{aligned}
E(S(G_{n+1})) =& E(S(G_n)) + 18B_n + 8A_n + 824n + 248 \\
=& E(S(G_n)) + 18[(20 - 12p_1 - 8p_2 - 4p_3)n^2 + (12p_1 + 8p_2 + 4p_3 - 4)n] \\
&+ 8[(45 - 27p_1 - 18p_2 - 9p_3)n^2 + (27p_1 + 18p_2 + 9p_3 - 14)n + 1] + 824n + 248,
\end{aligned}$$

and the boundary condition is $E(S(G_1)) = 256$.

According to the above recurrence relation and the boundary condition, we have

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

(1.7) holds. This completes the proof. $\square$

Specially, if $p_1 = 1$, which implies $p_2 = p_3 = p_4 = 0$, that is, $(p_1,\ p_2,\ p_3,\ p_4) = (1,0,0,0)$, then $G_n \cong M_n$. Similarly, if we take $(p_1,\ p_2,\ p_3,\ p_4) = (0,1,0,0)$ (resp. $(0,0,1,0)$, $(0,0,0,1)$), then $G_n \cong O_n^1$ (resp. $G_n \cong O_n^2$, $G_n \cong L_n$). By (1.6) and (1.7) in Theorem 1.1 we can receive the Gutman indices and the Schultz indices of the meta-chain M_n, the ortho-chain O_n^1, O_n^2, the para-chain L_n, as

$$\begin{aligned} Gut(M_n) &= 108n^3 + 396n^2 - 247n - 1, \quad Gut(O_n^1) = 162n^3 + 234n^2 - 139n - 1,\\ Gut(O_n^2) &= 216n^3 + 72n^2 - 31n - 1, \qquad Gut(L_n) = 270n^3 - 90n^2 + 77n - 1 \end{aligned}$$

and

$$\begin{aligned} S(M_n) &= 96n^3 + 392n^2 - 232n, \quad S(O_n^1) = 144n^3 + 248n^2 - 136n,\\ S(O_n^2) &= 192n^3 + 104n^2 - 40n, \quad S(L_n) = 240n^3 - 40n^2 + 56n, \end{aligned}$$

respectively. Furthermore, by direct calculation one has

$$Gut(M_n) + Gut(L_n) = Gut(O_n^1) + Gut(O_n^2), \quad S(M_n) + S(L_n) = S(O_n^1) + S(O_n^2).$$

3. Proofs of (1.8) and (1.9) in Theorem 1.1

In order to prove Theorem 1.1, it suffices to prove that (1.8) and (1.9) hold. In this section, we give the proofs of them. Consider the resistance distance between a vertex in V_{G_n} and a vertex in $V_{H_{n+1}}$, for any $v \in V_{G_n}$, one has

$$r(x_1,v) = r(u_n,v)+1,\ r(x_2,v) = r(u_n,v)+1+\frac{7}{8},\ r(x_3,v) = r(u_n,v)+1+\frac{12}{8},\ r(x_4,v) = r(u_n,v)+1+\frac{15}{8}, \tag{3.1}$$

$$r(x_5,v) = r(u_n,v)+1+\frac{16}{8}, r(x_6,v) = r(u_n,v)+1+\frac{15}{8}, r(x_7,v) = r(u_n,v)+1+\frac{12}{8}, r(x_8,v) = r(u_n,v)+1+\frac{7}{8}. \tag{3.2}$$

$$\sum_{v\in V_{G_n}} d_{G_{n+1}}(v) = 18n - 1. \tag{3.3}$$

Consider the resistance distance between two vertices in $V_{H_{n+1}}$, one has

$$\sum_{i=1}^{8} d(x_i)r(x_1,x_i) = 21,\ \sum_{i=1}^{8} d(x_i)r(x_2,x_i) = \frac{175}{8},\ \sum_{i=1}^{8} d(x_i)r(x_3,x_i) = \frac{45}{2},\ \sum_{i=1}^{8} d(x_i)r(x_4,x_i) = \frac{183}{8}, \tag{3.4}$$

$$\sum_{i=1}^{8} d(x_i)r(x_5,x_i) = 23,\ \sum_{i=1}^{8} d(x_i)r(x_6,x_i) = \frac{183}{8},\ \sum_{i=1}^{8} d(x_i)r(x_7,x_i) = \frac{45}{2},\ \sum_{i=1}^{8} d(x_i)r(x_8,x_i) = \frac{175}{8}. \tag{3.5}$$

Firstly, we prove that (1.8) holds. By (1.4), one has

$$Kf^*(G_{n+1}) = \sum_{\{u,v\}\subseteq V_{G_n}} d(u)d(v)r(u,v) + \sum_{v\in V_{G_n}} \sum_{x_i\in V_{H_{n+1}}} d(v)d(x_i)r(v,x_i) + \sum_{\{x_i,x_j\}\subseteq V_{H_{n+1}}} d(x_i)d(x_j)r(x_i,x_j).$$

By a similar discussion as the proof of (1.6) and (1.7), one has

$$\begin{aligned} \sum_{\{u,v\}\subseteq V_{G_n}} d(u)d(v)r(u,v) &= \sum_{\{u,v\}\subseteq V_{G_n}\setminus\{u_n\}} d(u)d(v)r(u,v) + \sum_{v\in V_{G_n}\setminus\{u_n\}} d_{G_{n+1}}(u_n)d(v)r(u_n,v)\\ &= \sum_{\{u,v\}\subseteq V_{G_n}\setminus\{u_n\}} d(u)d(v)r(u,v) + \sum_{v\in V_{G_n}\setminus\{u_n\}} (d_{G_n}(u_n)+1)d(v)r(u_n,v)\\ &= Kf^*(G_n) + \sum_{v\in V_{G_n}} d(v)r(u_n,v). \end{aligned}$$

Recall that $d(x_1) = 3$ and $d(x_i) = 2$ for $i \in \{2, 3, 4, 5, 6, 7, 8\}$. From(3.1)-(3.3), we have

$$\begin{aligned}
&\sum_{v \in V_{G_n}} \sum_{x_i \in V_{H_{n+1}}} d(v)d(x_i)r(v, x_i) \\
=&\sum_{v \in V_{G_n}} d(v)[3(r(u_n, v) + 1) + 2(r(u_n, v) + 1 + \frac{7}{8}) + 2(r(u_n, v) + 1 + \frac{12}{8}) + 2(r(u_n, v) + 1 + \frac{15}{8}) \\
&+ 2(r(u_n, v) + 1 + \frac{16}{8}) + 2(r(u_n, v) + 1 + \frac{15}{8}) + 2(r(u_n, v) + 1 + \frac{12}{8}) + 2(r(u_n, v) + 1 + \frac{7}{8})] \\
=&\sum_{v \in V_{G_n}} d(v)(17r(u_n, v) + 38) \\
=&17 \sum_{v \in V_{G_n}} d(v)r(u_n, v) + 38(18n - 1).
\end{aligned}$$

From(3.4)-(3.5), one has

$$\begin{aligned}
&\sum_{\{x_i, x_j\} \subseteq V_{H_{n+1}}} d(x_i)d(x_j)r(x_i, x_j) \\
=&\frac{1}{2} \sum_{i=1}^{8} d(x_i)(\sum_{j=1}^{8} d(x_j)r(x_i, x_j)) \\
=&\frac{1}{2}[3 \times 21 + 2 \times \frac{175}{8} + 2 \times \frac{45}{2} + 2 \times \frac{183}{8} + 2 \times 23 + 2 \times 3\frac{183}{8} + 2 \times \frac{45}{2} + 2 \times \frac{175}{8}] \\
=&189.
\end{aligned}$$

Then

$$Kf^*(G_{n+1}) = Kf^*(G_n) + 18 \sum_{v \in V_{G_n}} d(v)r(u_n, v) + 684n + 151. \tag{3.6}$$

For a random cyclooctatetraene chain G_n, the number $\sum_{v \in V_{G_n}} d(v)r(u_n, v)$ is a random variable. We may denote its expected value by

$$R_n := E(\sum_{v \in V_{G_n}} d(v)r(u_n, v)).$$

By direct calculation and (3.6), we can obtain a recurrence relation for the expected values of the multiplicative degree-Kirchhoff index of a random cyclooctatetraene chain G_n as follows,

$$E(Kf^*(G_{n+1})) = E(Kf^*(G_n)) + 18R_n + 684n + 151.$$

Considering the following four possible cases.

Case1. $G_n \longrightarrow G^1_{n+1}$. In this case, u_n is the vertex x_2 or x_8. Consequently, $\sum_{v \in V_{G_n}} d(v)r(u_n, v)$ is given by $\sum_{v \in V_{G_n}} d(v)r(x_2, v)$ or $\sum_{v \in V_{G_n}} d(v)r(x_8, v)$ with probability p_1.

Case2. $G_n \longrightarrow G^2_{n+1}$. In this case, u_n is the vertex x_3 or x_7. Consequently, $\sum_{v \in V_{G_n}} d(v)r(u_n, v)$ is given by $\sum_{v \in V_{G_n}} d(v)r(x_3, v)$ or $\sum_{v \in V_{G_n}} d(v)r(x_7, v)$ with probability p_2.

Case3. $G_n \longrightarrow G^3_{n+1}$. In this case, u_n is the vertex x_4 or x_6. Consequently, $\sum_{v \in V_{G_n}} d(v)r(u_n, v)$ is given by $\sum_{v \in V_{G_n}} d(v)r(x_4, v)$ or $\sum_{v \in V_{G_n}} d(v)r(x_6, v)$ with probability p_3.

Case4. $G_n \longrightarrow G^4_{n+1}$. In this case, u_n is the vertex x_5. Consequently, $\sum_{v \in V_{G_n}} d(v)r(u_n, v)$ is given by $\sum_{v \in V_{G_n}} d(v)r(x_5, v)$ with probability $1 - p_1 - p_2 - p_3$.

According to the above four cases, we may obtain the expected value R_n as

$$\begin{aligned}R_n =&p_1\sum_{v\in V_{G_n}} d(v)r(x_2,v)+p_2\sum_{v\in V_{G_n}} d(v)r(x_3,v)+p_3\sum_{v\in V_{G_n}} d(v)r(x_4,v)+(1-p_1-p_2-p_3)\sum_{v\in V_{G_n}} d(v)r(x_5,v)\\ =&p_1[\sum_{v\in V_{G_{n-1}}} d(v)r(u_{n-1},v)+(1+\frac{7}{8})(18n-19)+\frac{175}{8}]\\ &+p_2[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1},v)+(1+\frac{12}{8})(18n-19)+\frac{45}{2}]\\ &+p_3[\sum_{v\in V_{G_{n-1}}} d(v)d(u_{n-1},v)+(1+\frac{15}{8})(18n-19)+\frac{183}{8}]\\ &+(1-p_1-p_2-p_3)[\sum_{v\in V_{G_{n-1}}} d(v)r(u_{n-1},v)+(1+\frac{16}{8})(18n-19)+23].\end{aligned}$$

By applying the expected operator to the above equation, and noting that $E(R_n)=R_n$, we obtain

$$R_n=R_{n-1}+(54-\frac{81}{4}p_1-9p_2-\frac{9}{4}p_3)n+\frac{81}{4}p_1+9p_2+\frac{9}{4}p_3-34.$$

The boundary condition is

$$R_1=E(\sum_{v\in V_{G_1}} d(v)r(u_1,v))=21.$$

According to the above recurrence relation and the boundary condition, we have

$$R_n=(27-\frac{81}{8}p_1-\frac{9}{2}p_2-\frac{9}{8}p_3)n^2+(\frac{81}{8}p_1+\frac{9}{2}p_2+\frac{9}{8}p_3-7)n+1.$$

Therefore,

$$\begin{aligned}E(Kf^*(G_{n+1}))&=E(Kf^*(G_n))+18R_n+684n+151\\ &=E(Kf^*(G_n))+18[(27-\frac{81}{8}p_1-\frac{9}{2}p_2-\frac{9}{8}p_3)n^2+(\frac{81}{8}p_1+\frac{9}{2}p_2+\frac{9}{8}p_3-7)n+1]+684n+151,\end{aligned}$$

and the boundary condition is $E(Kf^*(G_1))=168$.

According to the above recurrence relation and the boundary condition, we have

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

(1.8) holds.

Now, we prove that (1.9) holds. By (1.5), one has

$$\begin{aligned}Kf^+(G_{n+1})=&\sum_{\{u,v\}\subseteq V_{G_n}}(d(u)+d(v))r(u,v)+\sum_{v\in V_{G_n}}\sum_{x_i\in V_{H_{n+1}}}(d(v)+d(x_i))r(v,x_i)\\ &+\sum_{\{x_i,x_j\}\subseteq V_{H_{n+1}}}(d(x_i)+d(x_j))r(x_i,x_j).\end{aligned}$$

By a similar discussion as above, one has

$$\begin{aligned}\sum_{\{u,v\}\subseteq V_{G_n}}(d(u)+d(v))r(u,v)=&\sum_{\{u,v\}\subseteq V_{G_n}\backslash\{u_n\}}(d(u)+d(v))r(u,v)+\sum_{v\in V_{G_n}\backslash\{u_n\}}(d_{G_{n+1}}(u_n)+d(v))r(u_n,v)\\ =&\sum_{\{u,v\}\subseteq V_{G_n}\backslash\{u_n\}}(d(u)+d(v))r(u,v)+\sum_{v\in V_{G_n}\backslash\{u_n\}}(d_{G_n}(u_n)+1+d(v))r(u_n,v)\\ =&Kf^+(G_n)+\sum_{v\in V_{G_n}} r(u_n,v).\end{aligned}$$

Recall that $d(x_1)=3$ and $d(x_i)=2$ for $i\in\{2,3,4,5,6,7,8\}$. From(3.1)-(3.3), we have

$$\begin{aligned}
&\sum_{v\in V_{G_n}}\sum_{x_i\in V_{H_{n+1}}}(d(v)+d(x_i))r(v,x_i)\\
=&\sum_{v\in V_{G_n}}\sum_{x_i\in V_{H_{n+1}}}d(v)r(v,x_i)+\sum_{v\in V_{G_n}}\sum_{x_i\in V_{H_{n+1}}}d(x_i)r(v,x_i)\\
=&\sum_{v\in V_{G_n}}d(v)[(r(u_n,v)+1)+(r(u_n,v)+1+\frac{7}{8})+(r(u_n,v)+1+\frac{12}{8})+(r(u_n,v)+1+\frac{15}{8})\\
&+(r(u_n,v)+1+\frac{16}{8})+(r(u_n,v)+1+\frac{15}{8})+(r(u_n,v)+1+\frac{12}{8})+(r(u_n,v)+1+\frac{7}{8})]\\
&+\sum_{v\in V_{G_n}}[3(r(u_n,v)+1)+2(r(u_n,v)+1+\frac{7}{8})+2(r(u_n,v)+1+\frac{12}{8})+2(r(u_n,v)+1+\frac{15}{8})\\
&+2(r(u_n,v)+1+\frac{16}{8})+2(r(u_n,v)+1+\frac{15}{8})+2(r(u_n,v)+1+\frac{12}{8})+2(r(u_n,v)+1+\frac{7}{8})]\\
=&8\sum_{v\in V_{G_n}}d(v)r(u_n,v)+\frac{37}{2}(18n-1)+17\sum_{v\in V_{G_n}}r(u_n,v)+38\times 8n.
\end{aligned}$$

Note that $\sum_{i=1}^{8}r(x_k,x_i)=\frac{21}{2}$ for $k=1,2,3,4,5,6,7,8$. From(3.4)-(3.5), one has

$$\begin{aligned}
\sum_{\{x_i,x_j\}\subseteq V_{H_{n+1}}}(d(x_i)+d(x_j))r(x_i,x_j)=&\frac{1}{2}\sum_{i=1}^{8}\sum_{j=1}^{8}(d(x_i)+d(x_j))r(x_i,x_j)\\
=&\sum_{i=1}^{8}\sum_{j=1}^{8}d(x_i)r(x_i,x_j)=\frac{21}{2}\times(3+2\times 7)\\
=&\frac{357}{2}.
\end{aligned}$$

Then

$$Kf^+(G_{n+1})=Kf^+(G_n)+18\sum_{v\in V_{G_n}}r(u_n,v)+8\sum_{v\in V_{G_n}}d(v)r(u_n,v)+637n+160. \tag{3.7}$$

For a random cyclooctatetraene chain G_n, the number $\sum_{v\in V_{G_n}}r(u_n,v)$ is a random variable. We may denote its expected value by

$$D_n:=E(\sum_{v\in V_{G_n}}r(u_n,v)).$$

By a direct calculation and (3.7), we can obtain a recurrence relation for the expected values of the additive degree-Kirchhoff index index of a random cyclooctatetraene chain G_n as follows,

$$E(Kf^+(G_{n+1}))=E(Kf^+(G_n))+18D_n+8R_n+637n+160.$$

Considering the following four possible cases.
Case1. $G_n\longrightarrow G_{n+1}^1$. In this case, u_n is the vertex x_2 or x_8. Consequently, $\sum_{v\in V_{G_n}}r(u_n,v)$ is given by $\sum_{v\in V_{G_n}}r(x_2,v)$ or $\sum_{v\in V_{G_n}}r(x_8,v)$ with probability p_1.
Case2. $G_n\longrightarrow G_{n+1}^2$. In this case, u_n is the vertex x_3 or x_7. Consequently, $\sum_{v\in V_{G_n}}r(u_n,v)$ is given by $\sum_{v\in V_{G_n}}r(x_3,v)$ or $\sum_{v\in V_{G_n}}r(x_7,v)$ with probability p_2.
Case3. $G_n\longrightarrow G_{n+1}^3$. In this case, u_n is the vertex x_4 or x_6. Consequently, $\sum_{v\in V_{G_n}}r(u_n,v)$ is given by $\sum_{v\in V_{G_n}}r(x_4,v)$ or $\sum_{v\in V_{G_n}}r(x_6,v)$ with probability p_3.
Case4. $G_n\longrightarrow G_{n+1}^4$. In this case, u_n is the vertex x_5. Consequently, $\sum_{v\in V_{G_n}}r(u_n,v)$ is given by $\sum_{v\in V_{G_n}}r(x_5,v)$ with probability $1-p_1-p_2-p_3$.

According to the above four cases, we may obtain the expected value D_n as

$$\begin{aligned}D_n =& p_1 \sum_{v\in V_{G_n}} r(x_2,v) + p_2 \sum_{v\in V_{G_n}} r(x_3,v) + p_3 \sum_{v\in V_{G_n}} r(x_4,v) + (1-p_1-p_2-p_3) \sum_{v\in V_{G_n}} r(x_5,v)\\ =& p_1[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{7}{8})\times 8(n-1) + \frac{21}{2}]\\ &+ p_2[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{12}{8})\times 8(n-1) + \frac{21}{2}]\\ &+ p_3[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{15}{8})\times 8(n-1) + \frac{21}{2}]\\ &+ (1-p_1-p_2-p_3)[\sum_{v\in V_{G_{n-1}}} r(u_{n-1},v) + (1+\frac{16}{8})\times 8(n-1) + \frac{21}{2}]\end{aligned}$$

By applying the expected operator to the above equation, and noting that $E(D_n) = D_n$, we obtain

$$D_n = D_{n-1} + (24 - 9p_1 - 4p_2 - p_3)n + 9p_1 + 4p_2 + p_3 - \frac{27}{2}.$$

The boundary condition is

$$D_1 = E(\sum_{v\in V_{G_1}} r(u_1,v)) = \frac{21}{2}.$$

According to the above recurrence relation and the boundary condition, we have

$$D_n = (12 - \frac{9}{2}p_1 - 2p_2 - \frac{1}{2}p_3)n^2 + (\frac{9}{2}p_1 + 2p_2 + \frac{1}{2}p_3 - \frac{3}{2})n,$$

and

$$R_n = (27 - \frac{81}{8}p_1 - \frac{9}{2}p_2 - \frac{9}{8}p_3)n^2 + (\frac{81}{8}p_1 + \frac{9}{2}p_2 + \frac{9}{8}p_3 - 7)n + 1.$$

Therefore,

$$\begin{aligned}E(Kf^+(G_{n+1})) =& E(Kf^+(G_n)) + 18D_n + 8R_n + 637n + 160\\ =& E(Kf^+(G_n)) + 18[(12 - \frac{9}{2}p_1 - 2p_2 - \frac{1}{2}p_3)n^2 + (\frac{9}{2}p_1 + 2p_2 + \frac{1}{2}p_3 - \frac{3}{2})n]\\ &+ 8[(27 - \frac{81}{8}p_1 - \frac{9}{2}p_2 - \frac{9}{8}p_3)n^2 + (\frac{81}{8}p_1 + \frac{9}{2}p_2 + \frac{9}{8}p_3 - 7)n + 1] + 637n + 160,\end{aligned}$$

and the boundary condition is $E(Kf^+(G_1)) = 168$.

According to the above recurrence relation and the boundary condition, we have

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

as desired. This completes the proof. □

Specially, if $(p_1,\ p_2,\ p_3,\ p_4) = (1,0,0,0)$(resp. $(0,1,0,0)$, $(0,0,1,0)$, $(0,0,0,1)$), then $G_n \cong M_n$ (resp. $G_n \cong O_n^1$, $G_n \cong O_n^2$, $G_n \cong L_n$). By (1.8) and (1.9) in Theorem 1.1 we can receive the multiplicative degree-Kirchhoff indices and the additive degree-Kirchhoff indices of the meta-chain M_n, the ortho-chain O_n^1, O_n^2, the para-chain L_n, as

$$\begin{aligned}Kf^*(M_n) &= \frac{405}{4}n^3 + \frac{873}{4}n^2 - \frac{301}{2}n - 1,\ Kf^*(O_n^1) = 135n^3 + 117n^2 - 83n - 1,\\ Kf^*(O_n^2) &= \frac{621}{4}n^3 + \frac{225}{4}n^2 - \frac{85}{2}n - 1, \quad Kf^*(L_n) = 162n^3 + 36n^2 - 29n - 1.\end{aligned}$$

and

$$\begin{aligned}Kf^+(M_n) &= 90n^3 + 223n^2 - 145n,\ Kf^+(O_n^1) = 120n^3 + 133n^2 - 85n,\\ Kf^+(O_n^2) &= 138n^3 + 79n^2 - 49n, \quad Kf^+(L_n) = 144n^3 + 61n^2 - 37n.\end{aligned}$$

respectively.

4. Proof of Corollary 1.2

In this following, we prove that Corollary 1.2 holds. By Theorem 1.1, we have

$$\begin{aligned}
E(Gut(G_n)) &= (-162n^3+486n^2-324n)p_1+(-108n^3+324n^2-216n)p_2+(-54n^3+162n^2-108n)p_3 \\
&\quad +270n^3-90n^2+77n-1; \qquad (4.1)\\
E(S(G_n)) &= (-144n^3+432n^2-288n)p_1+(-96n^3+288n^2-192n)p_2+(-48n^3+144n^2-96n)p_3 \\
&\quad +240n^3-40n^2+56n.; \qquad (4.2)\\
E(Kf^*(G_n)) &= (-\frac{243}{4}n^3+\frac{729}{4}n^2-\frac{243}{2}n)p_1+(-27n^3+81n^2-54n)p_2+(-\frac{27}{4}n^3+\frac{81}{4}n^2-\frac{27}{2}n)p_3 \\
&\quad +162n^3+36n^2-29n-1; \qquad (4.3)\\
E(Kf^+(G_n)) &= (-54n^3+162n^2-108n)p_1+(-24n^3+72n^2-48n)p_2+(-6n^3+18n^2-12n)p_3 \\
&\quad +144n^3+61n^2-37n. \qquad (4.4)
\end{aligned}$$

In order to prove Corollary 1.2, it suffices to prove the following four claims.

Claim 1. *For a random cyclooctatetraene chain G_n ($n \geq 3$), the para-chain L_n realizes the maximum of $E(Gut(G_n))$ and the meta-chain M_n realizes that of minimum.*

Proof. By (4.1), $E(Gut(G_n))$ may be seen as a function on p_1, p_2 and p_3 with $0 \leq p_i \leq 1$ for $i = 1, 2, 3$ and $p_1 + p_2 + p_3 \leq 1$. Note that $n \geq 3$, by taking the partial derivative, one has

$$\begin{aligned}
\frac{\partial E(Gut(G_n))}{\partial p_1} &= -162n^3+486n^2-324n<0,\\
\frac{\partial E(Gut(G_n))}{\partial p_2} &= -108n^3+324n^2-216n<0,\\
\frac{\partial E(Gut(G_n))}{\partial p_3} &= -54n^3+162n^2-108n<0.
\end{aligned}$$

If $p_1 = p_2 = p_3 = 0$ (i.e. $p_4 = 1$), the para-chain L_n realizes the maximum of $E(Gut(G_n))$, that is $G_n \cong L_n$.

If $p_1 + p_2 + p_3 = 1$, then $E(Gut(G_n))$ attains the minimum value, where $0 \leq p_i \leq 1$ for $i = 1, 2, 3$. Let $p_3 = 1 - p_1 - p_2$, we have

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

Therefore,

$$\frac{\partial E(Gut(G_n))}{\partial p_1} = -108n^3+324n^2-216n<0, \qquad \frac{\partial E(Gut(G_n))}{\partial p_2} = -54n^3+162n^2-108n<0.$$

Recall that $p_1 + p_2 + p_3 = 1$ and $0 \leq p_i \leq 1$ for $i = 1, 2, 3$. One has $0 \leq p_1 + p_2 \leq 1$. Clearly, if $p_1 + p_2 = 1$, then $E(Gut(G_n))$ attains the minimum value, where $0 \leq p_i \leq 1$ for $i = 1, 2$. Let $p_1 = 1 - p_2$, we have

$$E(Gut(G_n)) =(-162n^3+486n^2-324n)(1-p_2)+(-108n^3+324n^2-216n)p_2+270n^3-90n^2+77n-1.$$

Thus,

$$\frac{\partial E(Gut(G_n))}{\partial p_2} = 54n^3-162n^2+108n>0.$$

When $p_2 = 0$ (*i.e.* $p_1 = 1$), $E(Gut(G_n))$ achieves the minimum value, that is, $G_n \cong M_n$.

This completes the proof of Claim 1. □

Claim 2. *For a random cyclooctatetraene chain G_n ($n \geq 3$), the para-chain L_n realizes the maximum of $E(S(G_n))$ and the meta-chain M_n realizes that of minimum.*

Proof. By (4.2), $E(S(G_n))$ may be seen as a function on p_1, p_2 and p_3 with $0 \leq p_i \leq 1$ for $i = 1, 2, 3$ and $p_1 + p_2 + p_3 \leq 1$. Note that $n \geq 3$, by direct calculation, one has

$$\begin{aligned}
\frac{\partial E(S(G_n))}{\partial p_1} &= -144n^3 + 432n^2 - 288n < 0, \\
\frac{\partial E(S(G_n))}{\partial p_2} &= -96n^3 + 288n^2 - 192n < 0, \\
\frac{\partial E(S(G_n))}{\partial p_3} &= -48n^3 + 144n^2 - 96n < 0.
\end{aligned}$$

If $p_1 = p_2 = p_3 = 0$ (i.e. $p_4 = 1$), the para-chain L_n realizes the maximum of $E(S(G_n))$, that is $G_n \cong L_n$.

If $p_1 + p_2 + p_3 = 1$, then $E(S(G_n))$ attains the minimum value, where $0 \leq p_i \leq 1$ for $i = 1, 2, 3$. Let $p_3 = 1 - p_1 - p_2$, we have

$$\begin{aligned}
E(S(G_n)) =&(-144n^3 + 432n^2 - 288n)p_1 + (-96n^3 + 288n^2 - 192n)p_2 \\
&+ (-48n^3 + 144n^2 - 96n)(1 - p_1 - p_2) + 240n^3 - 40n^2 + 56n.
\end{aligned}$$

Therefore,

$$\frac{\partial E(S(G_n))}{\partial p_1} = -96n^3 + 288n^2 - 192n < 0, \qquad \frac{\partial E(S(G_n))}{\partial p_2} = -48n^3 + 144n^2 - 96n < 0.$$

Recall that $p_1 + p_2 + p_3 = 1$ and $0 \leq p_i \leq 1$ for $i = 1, 2, 3$. One has $0 \leq p_1 + p_2 \leq 1$. Clearly, if $p_1 + p_2 = 1$, then $E(S(G_n))$ attains the minimum value, where $0 \leq p_i \leq 1$ for $i = 1, 2$. Let $p_1 = 1 - p_2$, we have

Thus,

$$\frac{\partial E(S(G_n))}{\partial p_2} = 48n^3 - 144n^2 + 96n > 0.$$

When $p_2 = 0$ (*i.e.* $p_1 = 1$), $E(S(G_n))$ attains the minimum value, that is, $G_n \cong M_n$.

This completes the proof of Claim 2. □

Claim 3. *For a random cyclooctatetraene chain G_n ($n \geq 3$), the para-chain L_n realizes the maximum of $E(Kf^*(G_n))$ and the meta-chain M_n realizes that of minimum.*

Proof. By (4.3), $E(Kf^*(G_n))$ may be seen as a function on p_1, p_2 and p_3 with $0 \leq p_i \leq 1$ for $i = 1, 2, 3$ and $p_1 + p_2 + p_3 \leq 1$. Note that $n \geq 3$, by taking the partial derivative, one has

$$\begin{aligned}
\frac{\partial E(Kf^*(G_n))}{\partial p_1} &= -\frac{243}{4}n^3 + \frac{729}{4}n^2 - \frac{243}{2}n < 0, \\
\frac{\partial E(Kf^*(G_n))}{\partial p_2} &= -27n^3 + 81n^2 - 54n < 0, \\
\frac{\partial E(Kf^*(G_n))}{\partial p_3} &= -\frac{27}{4}n^3 + \frac{81}{4}n^2 - \frac{27}{2}n < 0.
\end{aligned}$$

If $p_1 = p_2 = p_3 = 0$ (i.e. $p_4 = 1$), the para-chain L_n realizes the maximum of $E(Kf^*(G_n))$, that is $G_n \cong L_n$.

If $p_1 + p_2 + p_3 = 1$, then $E(Kf^*(G_n))$ attains the minimum value, where $0 \leq p_i \leq 1$ for $i = 1, 2, 3$. Let $p_3 = 1 - p_1 - p_2$, we have

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

Hence,

$$\frac{\partial E(Kf^*(G_n))}{\partial p_1} = -54n^3 + 162n^2 - 108n < 0, \qquad \frac{\partial E(Kf^*(G_n))}{\partial p_2} = -\frac{81}{4}n^3 + \frac{243}{4}n^2 - \frac{81}{2}n < 0.$$

Recall that $p_1+p_2+p_3=1$ and $0\le p_i\le 1$ for $i=1,2,3$. One has $0\le p_1+p_2\le 1$. Clearly, if $p_1+p_2=1$, then $E(Kf^*(G_n))$ attains the minimum value, where $0\le p_i\le 1$ for $i=1,2$. Let $p_1=1-p_2$, we have

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

Thus,

$$\frac{\partial E(Kf^*(G_n))}{\partial p_2}=\frac{135}{4}n^3-\frac{405}{4}n^2+\frac{135}{2}n>0.$$

When $p_2=0$ (*i.e.* $p_1=1$), $E(Kf^*(G_n))$ achieves the minimum value, that is $G_n\cong M_n$.

This completes the proof of Claim 3. □

Claim 4. *For a random cyclooctatetraene chain G_n $(n\ge 3)$, the para-chain L_n realizes the maximum of $E(Kf^+(G_n))$ and the meta-chain M_n realizes that of minimum.*

Proof. By (4.4), $E(Kf^+(G_n))$ may be seen as a function on p_1,p_2 and p_3 with $0\le p_i\le 1$ for $i=1,2,3$ and $p_1+p_2+p_3\le 1$. Note that $n\ge 3$, by a direct calculation, one has

$$\begin{aligned}\frac{\partial E(Kf^+(G_n))}{\partial p_1}&=-54n^3+162n^2-108n<0,\\ \frac{\partial E(Kf^+(G_n))}{\partial p_2}&=-24n^3+72n^2-48n<0,\\ \frac{\partial E(Kf^+(G_n))}{\partial p_3}&=-6n^3+18n^2-12n<0.\end{aligned}$$

If $p_1=p_2=p_3=0$ (i.e. $p_4=1$), the para-chain L_n realizes the maximum of $E(Kf^+(G_n))$, that is $G_n\cong L_n$.

If $p_1+p_2+p_3=1$, then $E(Kf^+(G_n))$ attains the minimum value, where $0\le p_i\le 1$ for $i=1,2,3$. Let $p_3=1-p_1-p_2$, we have

$$\begin{aligned}E(Kf^+(G_n)) =&(-54n^3+162n^2-108n)p_1+(-24n^3+72n^2-48n)p_2\\ &+(-6n^3+18n^2-12n)(1-p_1-p_2)+144n^3+61n^2-37n.\end{aligned}$$

Hence,

$$\frac{\partial E(Kf^+(G_n))}{\partial p_1}=-48n^3+144n^2-96n<0,\qquad \frac{\partial E(Kf^+(G_n))}{\partial p_2}=-18n^3+54n^2-36n<0.$$

Recall that $p_1+p_2+p_3=1$ and $0\le p_i\le 1$ for $i=1,2,3$. One has $0\le p_1+p_2\le 1$. Clearly, if $p_1+p_2=1$, then $E(Kf^+(G_n))$ attains the minimum value, where $0\le p_i\le 1$ for $i=1,2$. Let $p_1=1-p_2$, we have

$$E(Kf^+(G_n)) =(-54n^3+162n^2-108n)(1-p_2)+(-24n^3+72n^2-48n)p_2+144n^3+61n^2-37n.$$

Thus,

$$\frac{\partial E(Kf^+(G_n))}{\partial p_2}=30n^3-90n^2+60n>0.$$

When $p_2=0$ (*i.e.* $p_1=1$), $E(Kf^+(G_n))$ attains the minimum value, that is $G_n\cong M_n$. This completes the proof of Claim 3.

By Claims 1-4, this corollary holds. □

5. Concluding remarks

In this paper, we obtain the explicit analytical expressions for the expected values of the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of a random cyclooctatetraene chain with n octagons. We also get the average values of these four indices. All these results will contribute to the study of the Gutman index, Schultz index, multiplicative degree-Kirchhoff index and additive degree-Kirchhoff index of graphs.

In chemical graph theory, the matter of polygonal chain is being widely studied by researchers. The molecular structures of polygonal chemicals are various and its physicochemical properties also become more and more important, and refer to [8, 28, 33, 35]. It is possible to establish exact formulas for the expected values of some indices of a random polygon chain with n regular polygons.

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