Multiplicative Degree-Kirchhoff Index
of Random Polyphenyl Chains

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The multiplicative degree-Kirchhoff index of a connected graph is defined as the sum of the product of the resistance distances between all pairs of points and the degrees of corresponding point pairs in the graph. In this paper, we propose an exact formula to compute the expected value of the multiplicative degree-Kirchhoff index of a random polyphenyl chain. Furthermore its asymptotic property is also considered.

1.   Introduction

Polyphenyls and their derivatives, which are used in heat exchangers, drug synthesis, organic synthesis, and so on, have attracted the attention of researchers in various fields for many years. Spiro-based compounds are a very important class of cycloalkanes in organic chemistry. The function of a spiro union is to form a linkage between two rings in spiro compounds, which consists of a single atom common to both rings. A free spiro union forms a linkage, which is the only direct union between the rings. In the past, when chemists wanted to determine the relationship between the properties of a compound and its molecular structure, it was necessary to perform many experiments and obtain a large amount of data.[1] By using the spiro union compounds, materials, drugs, crystals, and compounds can be represented by graph structures called molecular graphs. Also, conducting polymers, such as polythiophene (PTh), polyaniline (Pani), polypyrrole (PPy), and their derivatives, have been used as the active layers of different gas sensors since the early 1980s.[2] The thermal and chemical stabilities of conducting polymers under ambient conditions have enhanced their utilization as active sensing layers deposited by either an in situ electrochemical reaction or a chemical reaction on an electrode or an electrode array. Therefore, conducting polymers can be used to fabricate gas sensor devices, which respond to and/or detect particular toxic gases and volatile organic compounds (VOCs). These devices are also used as ion-trapping devices at ambient temperature for quality control in production and for environmental remediation.[2,3] When conducting polymers are used in different sensor devices, their resistance is an important factor affecting their sensitivity.

Resistance distance is a distance function on a graph introduced by Klein and Randic, which is based on the theory of electrical networks. They found that a graphical distance can be used to indicate the effective resistance between pairs of vertices.[4,5] In recent years, resistance distance has been widely used in random walk, electronic engineering, complex network, and chemical graph theory, and is attracting the attention of many scholars worldwide.[6–10] The effective resistance between two nodes in an electrical network corresponds to the resistance distance $r(v_i, v_j)$ between two vertices of a graph. Let G be a graph with vertex set $\{v_1, v_2, ..., v_n\}$. The corresponding electrical network is obtained by replacing each edge of the graph with a fixed resistance (unit resistance). In the past, many researchers used the mathematical literature to study and calculate the resistance distance. Also, many studies were carried out to compute Kirchhoff indexes of specific classes of graphs, or to find bounds for Kirchhoff indexes of graphs and to characterize extremal graphs. For example, bicyclic and unicyclic graphs with extremal Kirchhoff indexes are characterized to obtain sharp bounds for Kirchhoff indexes of specific graphs. Throughout this study, we used a graph to model the molecular structure, in which each edge denotes a chemical bond and each vertex expresses an atom between two atoms.

2. Exact Definition of Multiplicative Degree-Kirchhoff Index

The multiplicative degree-Kirchhoff index of a connected graph is defined as the sum of the product of the resistance distances between all pairs of points and the degrees of corresponding point pairs in the graph.[7]

$$Kf^*(G) = \sum_{1 \leq i < j \leq n} d_i d_j r(v_i, v_j) = \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} d_i d_j r(v_i, v_j) = \frac{1}{2} \sum_{i=1}^{n} R_{D^*}(v_i | G) \qquad (1)$$

Here, $R_{D^*}(v_i | G) = \sum_{j=1}^{n} d_i d_j r(v_i, v_j)$. In this definition, $r(v_i, v_j) = 0$.

The multiplicative degree-Kirchhoff index is an important topological index (invariant) of a graph, which is generated from the molecular structure and is a way of numerizing the molecular structure. It also reflects the structural characteristics of the compound. Polyphenyls are a type of macrocyclic aromatic hydrocarbon, which have attracted the attention of many chemists.[11–13] Polyphenyl molecular graphs (or more precisely, graphs representing the carbon atoms) are called polyphenyl systems. If each vertex of a polyphenyl system lies in a hexagon and the graph obtained by contracting every hexagon to a vertex in the polyphenyl system is a path, we call this system a polyphenyl chain. Figure 1 shows the unique polyphenyl chains for $n = 1, 2$ and all the polyphenyl chains for $n = 3, 4$.

More generally, a polyphenyl chain PPC_n with n hexagons is regarded as a polyphenyl chain with $n - 1$ hexagons by adding a cutting edge to a new hexagon, as shown in Fig. 2.[1]

For $n \geq 3$, the terminal hexagon can be attached in three ways, and the three local arrangements are denoted as PPC_{n+1}^1, PPC_{n+2}^1, and PPC_{n+3}^1, as shown in Fig. 3.[1]

A random polyphenyl chain $PPC(n, p_1, p_2)$ with n hexagons is obtained by the stepwise addition of terminal hexagons. At each step ($k = 3, 4, ..., n$), a random selection is made from one
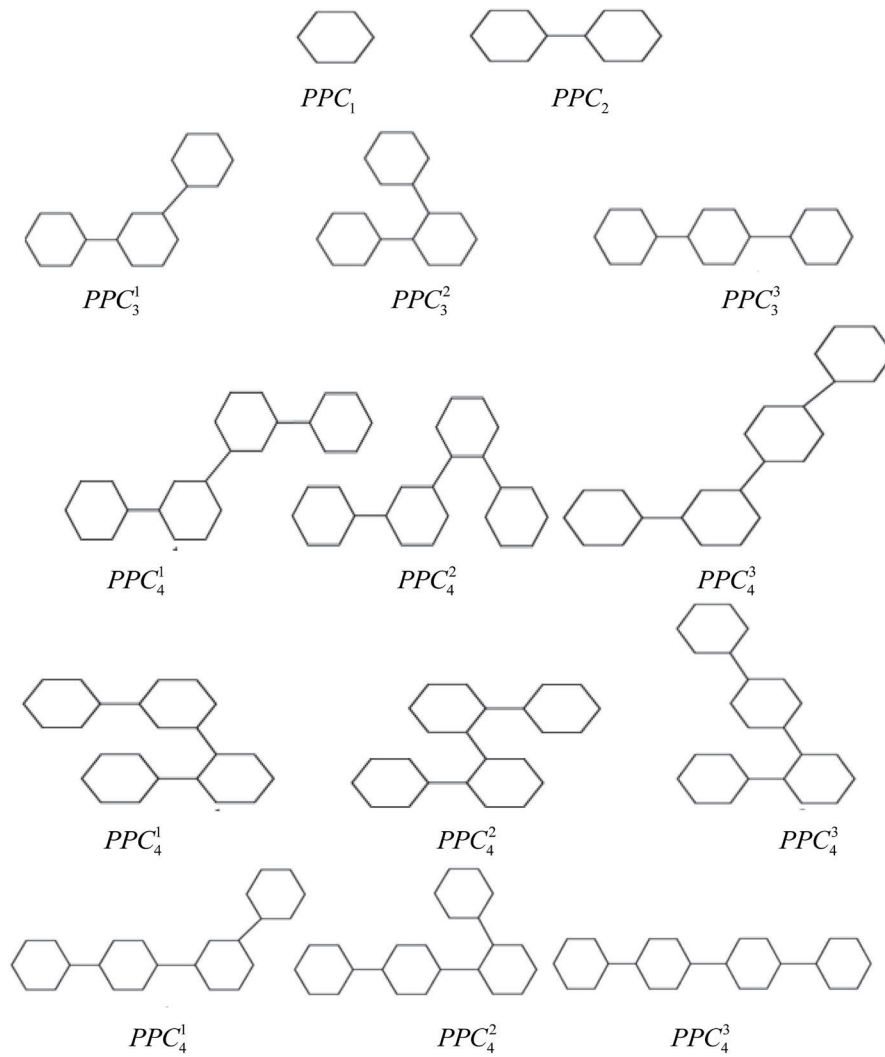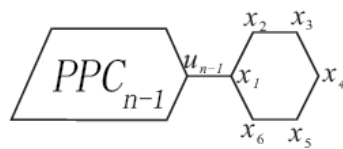
Fig. 1.   Polyphenyl chains.

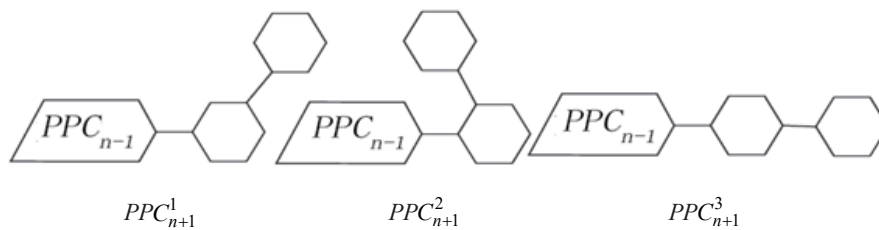Fig. 2.   Polyphenyl chain PPC_n with n hexagons.

Fig. 3.   Three local arrangements of polyphenyl chains.

of the three possible constructions: (1) $PPC_{k-1} \rightarrow PPC_k^1$ with probability p_1, (2) $PPC_{k-1} \rightarrow PPC_k^2$ with probability p_2, and (3) $PPC_{k-1} \rightarrow PPC_k^3$ with probability $p_3 = 1 - p_1 - p_2$. The important novelty of this study is we assume that probabilities p_1 and p_2 are constants and invariant with the step parameter k. For a random polyphenyl chain $PPC(n, p_1, p_2)$, the multiplicative degree-Kirchhoff index $Kf^*(PPC(n, p_1, p_2))$ is a random variable. Therefore, we propose an exact formula for its expected value $E(Kf^*(PPC(n, p_1, p_2)))$.

3. Main Result

Theorem 1: For $n \geq 1$, we have

$$
\begin{aligned}
E(Kf^*(PPC(n, p_1, p_2))) = 81\frac{2}{3} &- 13(29p_1 + 116p_2 - 406)\left[1 - \left(\frac{2}{3}\right)^{n-1}\right] \\
&+ \left[\frac{13}{3}(105 - 7p_1 - 28p_2) + \frac{518}{3}\right](n^2 + n - 2) \\
&+ (n-1)\left[\frac{13}{3}(57p_1 + 228p_2 - 826) - \frac{484}{3}\right].
\end{aligned}
\tag{2}
$$

Proof: As described above, the polyphenyl chain PPC_n is obtained by attaching PPC_{n-1} to a new terminal hexagon by a cutting edge, as shown in Fig. 2. If the terminal hexagon is spanned by vertices $x_1, x_2, ..., $ and x_6, then the new edge is denoted as $u_{n-1}x_1$, as shown in Fig. 2. Note that

1.

$$
\begin{aligned}
&d_1 d_2 r(x_1, x_2) = 3 \cdot 2 \cdot \frac{5}{6} = 5, \; d_1 d_3 r(x_1, x_3) = 3 \cdot 2 \cdot \frac{4}{3} = 8, \; d_1 d_4 r(x_1, x_4) = 3 \cdot 2 \cdot \frac{3}{2} = 9, \\
&d_1 d_5 r(x_1, x_5) = 3 \cdot 2 \cdot \frac{4}{3} = 8, \; d_1 d_6 r(x_1, x_6) = 3 \cdot 2 \cdot \frac{5}{6} = 5.
\end{aligned}
\tag{3}
$$

Thus, we have $\sum_{j=1}^{6} d_1 d_j r(x_1, x_j) = 35$.

$$
\begin{aligned}
&\sum_{j=1}^{6} d_1 d_j r(x_1, x_j) = 35, \; d_2 d_1 r(x_2, x_1) = 2 \cdot 3 \cdot \frac{5}{6} = 5, \; d_2 d_3 r(x_1, x_3) = 2 \cdot 2 \cdot \frac{5}{6} = \frac{10}{3}, \\
&d_2 d_4 r(x_2, x_4) = 2 \cdot 2 \cdot \frac{4}{3} = \frac{16}{3}, \; d_2 d_5 r(x_2, x_5) = 2 \cdot 2 \cdot \frac{3}{2} = 6, \; d_2 d_6 r(x_2, x_6) = 2 \cdot 2 \cdot \frac{4}{3} = \frac{16}{3}.
\end{aligned}
\tag{4}
$$

So we have $\sum_{j=1}^{6} d_2 d_j r(x_2, x_j) = 25$.

$$
\begin{aligned}
&\sum_{j=1}^{6} d_2 d_j r(x_2, x_j) = 25, \; d_3 d_1 r(x_3, x_1) = 2 \cdot 3 \cdot \frac{4}{3} = 8, \; d_3 d_2 r(x_3, x_2) = 2 \cdot 2 \cdot \frac{5}{6} = \frac{10}{3}, \\
&d_3 d_4 r(x_3, x_4) = 2 \cdot 2 \cdot \frac{5}{6} = \frac{10}{3}, \; d_3 d_5 r(x_3, x_5) = 2 \cdot 2 \cdot \frac{4}{3} = \frac{16}{3}, \; d_3 d_6 r(x_3, x_6) = 2 \cdot 2 \cdot \frac{3}{2} = 6.
\end{aligned}
\tag{5}
$$

Thus, we have $\sum_{j=1}^{6} d_3 d_j r(x_3, x_j) = 26$.

$$\sum_{j=1}^{6} d_3 d_j r(x_2, x_j) = 26, \ d_4 d_1 r(x_4, x_1) = 2 \cdot 3 \cdot \frac{3}{2} = 9, \ d_4 d_2 r(x_4, x_2) = 2 \cdot 2 \cdot \frac{4}{3} = \frac{16}{3},$$

$$d_4 d_3 r(x_4, x_3) = 2 \cdot 2 \cdot \frac{5}{6} = \frac{10}{3}, \ d_4 d_5 r(x_4, x_5) = 2 \cdot 2 \cdot \frac{5}{6} = \frac{10}{3}, \ d_4 d_6 r(x_4, x_6) = 2 \cdot 2 \cdot \frac{4}{3} = \frac{16}{3}. \tag{6}$$

Also, we have $\sum_{j=1}^{6} d_4 d_j r(x_4, x_j) = 9 + \frac{52}{3}$.

By symmetry, we have

$$\sum_{j=1}^{6} d_5 d_j r(x_5, x_j) = \sum_{j=1}^{6} d_3 d_j r(x_3, x_j) = 26, \ \sum_{j=1}^{6} d_6 d_j r(x_6, x_j) = \sum_{j=1}^{6} d_2 d_j r(x_2, x_j) = 25. \tag{7}$$

Thus, we obtain $\sum_{i=1}^{6} \sum_{j=1}^{6} d_i d_j r(x_i, x_j) = 35 + 25 + 26 + 9 + \frac{52}{3} + 26 + 25 = 146 + \frac{52}{3}$.

2. PPC_{n-1} has $6(n-1)$ vertices.

3. $\forall v \in PPC_{n-1}$,

$$d_1 d_v r(x_1, v) = 3 d_v [r(u_{n-1}, v) + 1], \ d_2 d_v r(x_2, v) = 2 d_v \left[r(u_{n-1}, v) + 1 + \frac{5}{6} \right],$$

$$d_3 d_v r(x_3, v) = 2 d_v \left[r(u_{n-1}, v) + 1 + \frac{4}{3} \right], \ d_4 d_v r(x_4, v) = 2 d_v \left[r(u_{n-1}, v) + 1 + \frac{3}{2} \right], \tag{8}$$

$$d_5 d_v r(x_5, v) = 2 d_v \left[r(u_{n-1}, v) + 1 + \frac{4}{3} \right], \ d_6 d_v r(x_6, v) = 2 d_v \left[r(u_{n-1}, v) + 1 + \frac{5}{6} \right].$$

The product of degree x_1 in PPC_n is denoted by $R_{D^*}(x_1 | PPC_n)$, and we have

$$\begin{aligned} R_{D^*}(x_1 | PPC_n) &= \sum_{j \in PPC_n} d_1 d_j r(x_1, x_j) \\ &= \sum_{v \in PPC_{n-1}} d_1 d_v r(x_1, v) + d_1 d_2 r(x_1, x_2) + d_1 d_3 r(x_1, x_3) \\ &\quad + d_1 d_4 r(x_1, x_4) + d_1 d_5 r(x_1, x_5) + d_1 d_6 r(x_1, x_6) \\ &= \sum_{v \in PPC_{n-1}} 3 d_v [r(u_{n-1}, v) + 1] + 35. \end{aligned} \tag{9}$$

Similarly,

$$R_{D^*}(x_2 | PPC_n) = \sum_{v \in PPC_{n-1}} 2 d_v \left[r(u_{n-1}, v) + \frac{11}{6} \right] + 25, \tag{10}$$

$$R_{D^*}(x_3|PPC_n) = \sum_{v \in PPC_{n-1}} 2d_v\left[r(u_{n-1},v) + \frac{7}{3}\right] + 26, \tag{11}$$

$$R_{D^*}(x_4|PPC_n) = \sum_{v \in PPC_{n-1}} 2d_v\left[r(u_{n-1},v) + \frac{5}{2}\right] + 9 + \frac{52}{3}, \tag{12}$$

$$R_{D^*}(x_5|PPC_n) = \sum_{v \in PPC_{n-1}} 2d_v\left[r(u_{n-1},v) + \frac{7}{3}\right] + 26, \tag{13}$$

$$R_{D^*}(x_6|PPC_n) = \sum_{v \in PPC_{n-1}} 2d_v\left[r(u_{n-1},v) + \frac{11}{6}\right] + 25. \tag{14}$$

Also,

$$Kf^*(PPC_n) = Kf^*(PPC_{n-1}) + R_{D^*}(x_1|PPC_n) + R_{D^*}(x_2|PPC_n) + R_{D^*}(x_3|PPC_n)$$

$$+ R_{D^*}(x_4|PPC_n) + R_{D^*}(x_5|PPC_n) + R_{D^*}(x_6|PPC_n) - \frac{1}{2}\sum_{i=1}^{6}\sum_{j=1}^{6}d_i d_j r(x_i,x_j)$$

$$= Kf^*(PPC_{n-1}) + 13\sum_{v \in PPC_{n-1}} d_v r(u_{n-1},v) + \frac{74}{3}\sum_{v \in PPC_{n-1}} d_v + 73 + \frac{52}{6} \tag{15}$$

$$= Kf^*(PPC_{n-1}) + \frac{13}{3}\sum_{v \in PPC_{n-1}} d_{u_{n-1}} d_v r(u_{n-1},v) + \frac{74}{3}\sum_{v \in PPC_{n-1}} d_v + 73 + \frac{52}{6}$$

$$= Kf^*(PPC_{n-1}) + \frac{13}{3}R_{D^*}(u_{n-1}|PPC_{n-1}) + \frac{74}{3}(14n - 16) + 73 + \frac{52}{6}.$$

Then,

$$Kf^*(PPC_{n+1}) = Kf^*(PPC_n) + \frac{13}{3}R_{D^*}(u_n|PPC_n) + \frac{74}{3}\cdot(14n - 2) + 73 + \frac{52}{6}. \tag{16}$$

For a random polyphenyl chain $PPC(n, p_1, p_2)$, $R_{D^*}(u_n|PPC(n, p_1, p_2))$ is a random variable, and we denote its expected value by $U_n = E(R_{D^*}(u_n|PPC(n, p_1, p_2)))$. There are three cases to consider:

Case 1. $PPC_n \rightarrow PPC_{n+1}^1$. In this case, u_n coincides with the vertex labeled x_3 or x_5. Consequently, $R_{D^*}(u_n|PPC(n, p_1, p_2))$ is given by Eq. (11) or (13).

Case 2. $PPC_n \rightarrow PPC_{n+1}^2$. In this case, u_n coincides with the vertex labeled x_2 or x_6. Consequently, $R_{D^*}(u_n|PPC(n, p_1, p_2))$ is given by Eq. (10) or (14).

Case 3. $PPC_n \rightarrow PPC_{n+1}^3$. In this case, u_n coincides with the vertex labeled x_4. Consequently, $R_{D^*}(u_n|PPC(n, p_1, p_2))$ is given by Eq. (12).

Since the above three cases occur in random polyphenyl chains with probabilities p_1, p_2, and $1 - p_1 - p_2$, respectively, we immediately obtain the following result:

$$
\begin{aligned}
U_n &= E\left(R_{D^*}\left(u_n \middle| PPC(n, p_1, p_2)\right)\right) \\
&= p_1 \left\{ \sum_{v \in PPC_{n-1}} 2d_v \left[r(u_{n-1}, v) + \frac{7}{3} \right] + 26 \right\} + p_2 \left\{ \sum_{v \in PPC_{n-1}} 2d_v \left[r(u_{n-1}, v) + \frac{11}{6} \right] + 25 \right\} \\
&\quad + (1 - p_1 - p_2) \left\{ \sum_{v \in PPC_{n-1}} 2d_v \left[r(u_{n-1}, v) + \frac{5}{2} \right] + 9 + \frac{52}{3} \right\} \\
&= p_1 \left[\frac{2}{3} \sum_{v \in PPC_{n-1}} 3d_v r(u_{n-1}, v) + \frac{14}{3} \sum_{v \in PPC_{n-1}} d_v + 26 \right] \\
&\quad + p_2 \left[\frac{2}{3} \sum_{v \in PPC_{n-1}} 3d_v r(u_{n-1}, v) + \frac{11}{3} \sum_{v \in PPC_{n-1}} d_v + 25 \right] \\
&\quad + (1 - p_1 - p_2) \left[\frac{2}{3} \sum_{v \in PPC_{n-1}} 3d_v r(u_{n-1}, v) + 5 \sum_{v \in PPC_{n-1}} d_v + 9 + \frac{52}{3} \right] \\
&= p_1 \left[\frac{2}{3} R_{D^*}(u_{n-1} | PPC_{n-1}) + \frac{14}{3} \cdot (14n - 16) + 26 \right] \\
&\quad + p_2 \left[\frac{2}{3} R_{D^*}(u_{n-1} | PPC_{n-1}) + \frac{11}{3} \cdot (14n - 16) + 25 \right] \\
&\quad + (1 - p_1 - p_2) \left[\frac{2}{3} R_{D^*}(u_{n-1} | PPC_{n-1}) + 5 \cdot (14n - 16) + 9 + \frac{52}{3} \right].
\end{aligned}
\tag{17}
$$

By applying the properties of mathematical expectation to the above equation and noting that $E(U_n) = U_n$, we obtain

$$
\begin{aligned}
U_n &= p_1 \left[\frac{2}{3} U_{n-1} + \frac{14}{3} \cdot (14n - 16) + 26 \right] + p_2 \left[\frac{2}{3} U_{n-1} + \frac{11}{3} \cdot (14n - 16) + 25 \right] \\
&\quad + (1 - p_1 - p_2) \left[\frac{2}{3} U_{n-1} + 5 \cdot (14n - 16) + 9 + \frac{52}{3} \right].
\end{aligned}
\tag{18}
$$

This equation is easily transformed into

$$
U_n = \frac{2}{3} U_{n-1} + \left(70 - \frac{14}{3} p_1 - \frac{56}{3} p_2 \right) n + 5 p_1 + 20 p_2 - \frac{161}{3}.
\tag{19}
$$

The boundary condition is

$$
U_1 = E(R_{D^*}(u_1 | PPC(1, p_1, p_2))) = \sum_{j=1}^{6} d_1 d_j r(x_1, x_j) = 35.
\tag{20}
$$

Using the above recurrence relation and the boundary condition, we obtain the value of U_n.
Denoting $a = 70 - \dfrac{14}{3}p_1 - \dfrac{56}{3}p_2$, $b = 5p_1 + 20p_2 - \dfrac{161}{3}$, we have

$$U_n = \frac{2}{3}U_{n-1} + a \cdot n + b. \tag{21}$$

Denoting $d_1 = U_2 - U_1$, $d_2 = U_3 - U_2$, ..., $d_{n-1} = U_n - U_{n-1}$, we have

$$U_n = d_1 + d_2 + \cdots + d_{n-1} + U_1,$$
$$U_{n-1} = \frac{2}{3}U_{n-2} + a \cdot (n-1) + b. \tag{22}$$

By subtracting Eq. (22) from Eq. (21), we obtain

$$d_{n-1} = \frac{2}{3}d_{n-2} + a. \tag{23}$$

When $d_1 = U_2 - U_1 = \dfrac{2}{3} \cdot 35 + 2a + b - 35 = 2a + b - \dfrac{35}{3}$, from Eq. (23), we obtain

$$d_2 = \frac{2}{3}d_1 + a,\ d_3 = \frac{2}{3}d_2 + a = \frac{2}{3}\left(\frac{2}{3}d_1 + a\right) + a = \left(\frac{2}{3}\right)^2 d_1 + \left(1 + \frac{2}{3}\right)a,$$

$$d_4 = \left(\frac{2}{3}\right)^3 d_1 + \left[1 + \left(\frac{2}{3}\right) + \left(\frac{2}{3}\right)^2\right]a, ..., \tag{24}$$

$$d_{n-1} = \left(\frac{2}{3}\right)^{n-2} d_1 + \left[1 + \left(\frac{2}{3}\right) + \left(\frac{2}{3}\right)^2 + \cdots + \left(\frac{2}{3}\right)^{n-3}\right]a = \left(\frac{2}{3}\right)^{n-2} d_1 + 3a \cdot \left[1 - \left(\frac{2}{3}\right)^{n-2}\right]$$

Then,

$$U_n = d_1 + d_2 + \cdots + d_{n-1} + U_1$$

$$= 35 + \left[1 + \frac{2}{3} + \left(\frac{2}{3}\right)^2 + \cdots + \left(\frac{2}{3}\right)^{n-2}\right]d_1 + 3a \cdot \left\{\left(1 - \frac{2}{3}\right) + \left[1 - \left(\frac{2}{3}\right)^2\right] + \cdots + \left[1 - \left(\frac{2}{3}\right)^{n-2}\right]\right\}$$

$$= 35 + 3 \cdot \left[1 - \left(\frac{2}{3}\right)^{n-1}\right]d_1 + 3a\left\{n - 2 - \left[\frac{2}{3} + \left(\frac{2}{3}\right)^2 + \cdots + \left(\frac{2}{3}\right)^{n-2}\right]\right\} \tag{25}$$

$$= 35 + 3 \cdot \left[1 - \left(\frac{2}{3}\right)^{n-1}\right] \cdot \left(2a + b - \frac{35}{3}\right) + 3a\left\{(n-1) - 3\left[1 - \left(\frac{2}{3}\right)^{n-1}\right]\right\}$$

$$= 35 + \left[1 - \left(\frac{2}{3}\right)^{n-1}\right] \cdot (-3a + 3b - 35) + 3a(n-1).$$

Noting that $a = 70 - \dfrac{14}{3} p_1 - \dfrac{56}{3} p_2$, $b = 5 p_1 + 20 p_2 - \dfrac{161}{3}$, from Eq. (25), we obtain

$$U_n = 35 + (29 p_1 + 116 p_2 - 406) \left[1 - \left(\frac{2}{3} \right)^{n-1} \right] + (210 - 14 p_1 - 56 p_2)(n-1). \qquad (26)$$

Using the recurrence relation in Eq. (16), Eq. (26), and the expectation operator, we obtain

$$
\begin{aligned}
E(Kf^*(PPC(n, p_1, p_2))) &= E(Kf^*(PPC(n-1, p_1, p_2))) + \frac{13}{3} U_{n-1} + \frac{74}{3}(14n - 16) + 73 + \frac{52}{6} \\
&= E(Kf^*(PPC(n-1, p_1, p_2))) + \frac{74}{3}(14n - 16) + 73 + \frac{52}{6} \\
&\quad + \frac{13}{3} \left\{ 35 + (29 p_1 + 116 p_2 - 406)\left[1 - \left(\frac{2}{3}\right)^{n-2} \right] + (210 - 14 p_1 - 56 p_2)(n-2) \right\} \qquad (27) \\
&= E(Kf^*(PPC(n-1, p_1, p_2))) - \frac{13}{3}(29 p_1 + 116 p_2 - 406) \cdot \left(\frac{2}{3} \right)^{n-2} \\
&\quad + \left[\frac{13}{3}(210 - 14 p_1 - 56 p_2) + \frac{1036}{3} \right] n + \frac{13}{3}(57 p_1 + 228 p_2 - 826) - \frac{484}{3}.
\end{aligned}
$$

The boundary condition is $E(Kf^*(PPC(1, p_1, p_2))) = 73 + \dfrac{52}{6} = 81\dfrac{2}{3}$, and using the above recurrence relation and the boundary condition, we have

$$
\begin{aligned}
E(Kf^*(PPC(n, p_1, p_2))) &= 81\frac{2}{3} - 13(29 p_1 + 116 p_2 - 406)\left[1 - \left(\frac{2}{3}\right)^{n-1} \right] \\
&\quad + \left[\frac{13}{3}(210 - 14 p_1 + -56 p_2) + \frac{1036}{3} \right] \frac{n^2 + n - 2}{2} \\
&\quad + (n-1)\left[\frac{13}{3}\left(57 p_1 + 228 p_2 - \frac{484}{3} \right) \right] \\
&= 81\frac{2}{3} - 13(29 p_1 + 116 p_2 - 406)\left[1 - \left(\frac{2}{3}\right)^{n-1} \right] \\
&\quad + \left[\frac{13}{3}(105 - 7 p_1 - 28 p_2) + \frac{518}{3} \right](n^2 + n - 2) \\
&\quad + (n-1)\left[\frac{13}{3}(57 p_1 + 228 p_2 - 826) - \frac{484}{3} \right].
\end{aligned}
\qquad (28)
$$

Finally, we point out the asymptotic property of $E(Kf^*(PPC(n, p_1, p_2)))$, which is

$$E(Kf^*(PPC(n, p_1, p_2))) \sim \left[\frac{13}{3}(105 - 7 p_1 - 28 p_2) + \frac{518}{3} \right] n^2 \quad (n \to \infty). \qquad (29)$$

4.   Conclusions

The Kirchhoff index is not only an important invariant number characterizing bicyclic and unicyclic graphs, but is also an important means of describing molecular structures in chemistry. The Kirchhoff index also has important applications in the quantitative structure–activity relationships and quantitative structure–property relationships. It is very difficult to compute the Kirchhoff index from the computational complexity of the graph, and it is also difficult to obtain a specific formula for calculating the multiplicative degree-Kirchhoff index of a general graph. Therefore, the problem of finding the Kirchhoff index for some special graphs has attracted the widespread attention of researchers. In this study, we used the digital features of random variables and the methods and technologies of algebra to obtain the multiplicative degree-Kirchhoff index of a random polyphenyl chain. We also consider that the development potential nature of the Kirchhoff index in physics, chemistry, and other fields will have further applications.

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