



Research article

Topological indices of linear crossed phenylenes with respect to their Laplacian and normalized Laplacian spectrum

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Abstract: As a powerful tool for describing and studying the properties of networks, the graph spectrum analyses and calculations have attracted substantial attention from the scientific community. Let C_n represent linear crossed phenylenes. Based on the Laplacian (normalized Laplacian, resp.) polynomial of C_n , we first investigated the Laplacian (normalized Laplacian, resp) spectrum of C_n in this paper. Furthermore, the Kirchhoff index, multiplicative degree-Kirchhoff index and complexity of C_n were obtained through the relationship between the roots and the coefficients of the characteristic polynomials. Finally, it was found that the Kirchhoff index and multiplicative degree-Kirchhoff index of C_n were approximately one quarter of their Wiener index and Gutman index, respectively.

Keywords: Laplacian spectrum; normalized Laplacian spectrum; Kirchhoff index; multiplicative degree-Kirchhoff index; complexity

Mathematics Subject Classification: 05C50, 05C90

1. Introduction

In recent years, researchers have been interested in the study of complex networks [1–4]. Three common characteristics of complex networks are: small-world, scale-free, and fractal. Yang and Huang et al. [5, 6] have determined the Kirchhoff index and multiplicative degree-Kirchhoff index of hexagonal chains, and they obtained that the Kirchhoff index and multiplicative degree-Kirchhoff index of hexagonal chains are approximately half of their Wiener index and Gutman index, respectively. In particular, Peng et al. [7] studied the Kirchhoff index and complexity for linear phenylenes, and determined that the Kirchhoff index of linear phenylenes is approximately half of its Wiener index. In addition, Z. Zhu and J.-B. Liu [8] obtained the multiplicative degree-Kirchhoff index and complexity of generalized phenylenes. In 2018, Pan and Li [9] determined the Kirchhoff index, multiplicative degree-Kirchhoff index, and complexity of linear crossed hexagonal networks, and obtained that the Kirchhoff

index and multiplicative degree-Kirchhoff index of linear crossed hexagonal chains are approximately one quarter of their Wiener index and Gutman index, respectively. For other networks, see [10–14].

Motivated by these, we investigate the Laplacian and normalized Laplacian spectra of linear crossed phenylenes. We also obtain that the Kirchhoff index and multiplicative degree-Kirchhoff index of linear crossed phenylenes are approximately one quarter of their Wiener index and Gutman index, respectively.

In this paper, we suppose $G = (E_G, V_G)$ is a graph with edge set $E_G = \{e_1, e_2, \dots, e_m\}$ and vertex set $V_G = \{v_1, v_2, \dots, v_n\}$. For more notations, one can be referred to [15].

Let $D(G) = \text{diag}\{d_1, d_2, \dots, d_n\}$ represent a degree matrix, and $A(G)$ be the adjacency matrix, where d_i is the degree of v_i . Therefore, we can calculate the Laplacian matrix and normalized Laplacian matrix, which are defined as $L(G) = D(G) - A(G)$ and $\mathcal{L}(G) = D(G)^{-\frac{1}{2}}LD(G)^{-\frac{1}{2}}$, respectively. The Laplacian matrix is

$$(L(G))_{ij} = \begin{cases} d_i, & i = j; \\ -1, & i \neq j, v_i \text{ and } v_j \text{ are adjacent}; \\ 0, & \text{otherwise.} \end{cases} \quad (1.1)$$

The normalized Laplacian matrix is

$$(\mathcal{L}(G))_{ij} = \begin{cases} 1, & i = j, d_i \neq 0; \\ -\frac{1}{\sqrt{d_i d_j}}, & i \neq j, v_i \text{ and } v_j \text{ are adjacent}; \\ 0, & \text{otherwise.} \end{cases} \quad (1.2)$$

The *distance* between vertices v_i and v_j , denoted by d_{ij} , is defined as the length of the shortest path between vertices v_i and v_j . The *Wiener index* [16, 17] is defined as

$$W(G) = \sum_{i < j} d_{ij}. \quad (1.3)$$

In 1994, the *Gutman index* [18] is defined as

$$\text{Gut}(G) = \sum_{i < j} d_i d_j d_{ij}. \quad (1.4)$$

Klein and Randić [19] were the first to put forward the concept of *resistance distance*, and the *resistance distance* between vertices v_i and v_j is denoted by r_{ij} . Klein et al. [20, 21] introduced the *Kirchhoff index* as $Kf(G) = \sum_{i < j} r_{ij}$. In 2007, Chen et al. [22] proposed the *multiplicative degree-Kirchhoff index* as $Kf^*(G) = \sum_{i < j} d_i d_j r_{ij}$. Gutman and Mohar [23] introduced the *Kirchhoff index* as

$$Kf(G) = n \sum_{k=2}^n \frac{1}{\mu_k}, \quad (1.5)$$

where $0 = \mu_1 < \mu_2 \leq \dots \leq \mu_n (n \geq 2)$ are the eigenvalues of $L(G)$.

According to the normalized Laplacian, Chen et al. [22] proposed the *multiplicative degree-Kirchhoff index* as

$$Kf^*(G) = 2m \sum_{k=2}^n \frac{1}{\lambda_k}, \tag{1.6}$$

where $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ are the normalized Laplacian eigenvalues of $\mathcal{L}(G)$.

The *number of spanning trees* of G can also be called the *complexity* of G [15], denoted by $\tau(G)$.

In Section 2, we mainly introduce some notations and theorems. Next, applying the relationship between the roots and coefficients of C_n , the Laplacian spectrum of C_n is determined in Section 3. In Section 4, we obtain the normalized Laplacian spectrum of C_n in the same way as in Section 3. The conclusion is summarized in Section 5.

2. Preliminary

First, we state some notations and theorems, which will be used later.

Given an $n \times n$ matrix M , the submatrix of M is represented by $M[i_1, \dots, i_k]$, where $M[i_1, \dots, i_k]$ is formed by removing the i_1 -th, \dots , i_k -th rows and columns of M . Let $P_M(x) = \det(xI - M)$ represent the characteristic polynomial of M .

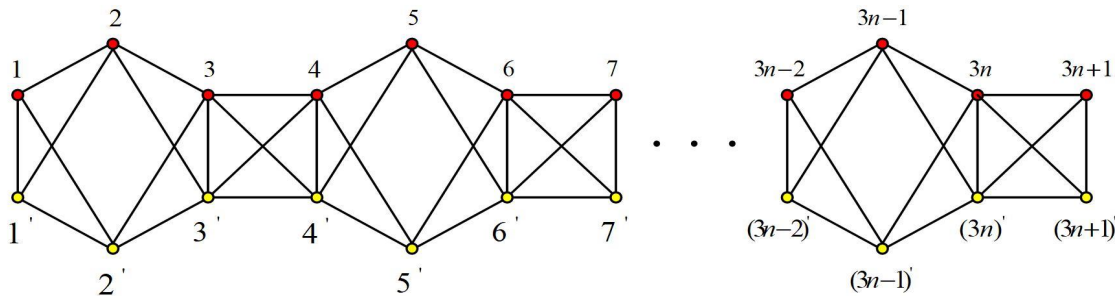


Figure 1. Linear crossed phenylenes C_n .

Label linear crossed phenylenes as shown in Figure 1. Evidently, $|V(C_n)| = 6n + 2$, $|E(C_n)| = 14n + 1$ and $\pi = (1, 1')(2, 2') \dots (3n + 1, (3n + 1)')$ is an automorphism of C_n . Set $V_1 = \{1, 2, \dots, 3n + 1\}$, $V_2 = \{1', 2', \dots, (3n + 1)'\}$.

Thus, $L(C_n)$ and $\mathcal{L}(C_n)$ can be expressed by

$$L(C_n) = \begin{pmatrix} L_{V_1V_1} & L_{V_1V_2} \\ L_{V_2V_1} & L_{V_2V_2} \end{pmatrix}, \quad \mathcal{L}(C_n) = \begin{pmatrix} \mathcal{L}_{V_1V_1} & \mathcal{L}_{V_1V_2} \\ \mathcal{L}_{V_2V_1} & \mathcal{L}_{V_2V_2} \end{pmatrix},$$

where

$$L_{V_1V_1} = L_{V_2V_2}, \quad L_{V_1V_2} = L_{V_2V_1}, \quad \mathcal{L}_{V_1V_1} = \mathcal{L}_{V_2V_2}, \quad \mathcal{L}_{V_1V_2} = \mathcal{L}_{V_2V_1}.$$

Let

$$T = \begin{pmatrix} \frac{1}{\sqrt{2}}I_{3n+1} & \frac{1}{\sqrt{2}}I_{3n+1} \\ \frac{1}{\sqrt{2}}I_{3n+1} & -\frac{1}{\sqrt{2}}I_{3n+1} \end{pmatrix},$$

Lemma 3.1. If $0 = \alpha_1 < \alpha_2 \leq \alpha_3 \leq \dots \leq \alpha_{3n+1}$ are the eigenvalues of L_A , one gets

$$\sum_{i=2}^{3n+1} \frac{1}{\alpha_i} = \frac{n(3n+2)}{4}.$$

Applying (3.1) - (3.2) and Lemma 3.1, we obtain the following theorem.

Theorem 3.2. For linear crossed phenylenes C_n , we have

$$Kf(C_n) = \frac{27n^3 + 48n^2 + 25n + 4}{6}.$$

The Kirchhoff indices of C_n are shown in Table 1, where $1 \leq n \leq 15$.

Table 1. Kirchhoff indices from C_1 to C_{15} .

G	$Kf(G)$	G	$Kf(G)$	G	$Kf(G)$	G	$Kf(G)$	G	$Kf(G)$
C_1	17.33	C_4	433.33	C_7	1965.33	C_{10}	5342.33	C_{13}	11293.33
C_2	77.00	C_5	784.00	C_8	2850.00	C_{11}	7004.00	C_{14}	13975.00
C_3	206.67	C_6	1285.67	C_9	3966.67	C_{12}	8978.67	C_{15}	17050.67

Theorem 3.3. Assume that C_n are the linear crossed phenylenes, then

$$\lim_{n \rightarrow \infty} \frac{Kf(C_n)}{W(C_n)} = \frac{1}{4}.$$

Proof. By first classifying and discussing the following cases of vertices, the Wiener index of C_n is obtained.

- Vertex $3j - 1$ ($j = 1, 2, \dots, n$) of C_n :

$$w_1(i) = 2 + 2 \left(\sum_{k=1}^{i-1} k + \sum_{k=1}^{3n+1-i} k \right), i = 3j - 1.$$

- Vertex $3j$ ($j = 1, 2, \dots, n$) of C_n :

$$w_2(i) = 1 + 2 \left(\sum_{k=1}^{i-1} k + \sum_{k=1}^{3n+1-i} k \right), i = 3j.$$

- Vertex $3j + 1$ ($j = 1, 2, \dots, n - 1$) of C_n :

$$w_3(i) = 1 + 2 \left(\sum_{k=1}^{i-1} k + \sum_{k=1}^{3n+1-i} k \right), i = 3j + 1.$$

- Vertex 1 of C_n :

$$w_4(i) = 1 + 2 \left(\sum_{k=1}^{3n} k \right).$$

Therefore, we need to calculate the first sum in (4.1).

Let

$$P_{\mathcal{L}_A}(x) = \det(xI - \mathcal{L}_A) = x^{3n+1} + b_1x^{3n} + \cdots + b_{3n}x.$$

Based on the Vieta's Theorem of $P_{\mathcal{L}_A}(x)$, we can get

$$\sum_{i=2}^{3n+1} \frac{1}{\gamma_i} = \frac{(-1)^{3n-1}b_{3n-1}}{(-1)^{3n}b_{3n}}. \quad (4.3)$$

Obviously, we obtain that $(-1)^{3n}b_{3n}$ is the sum of all the principal minors of order $3n$ of \mathcal{L}_A and $(-1)^{3n-1}b_{3n-1}$ is the sum of the principal minors of order $3n - 1$ of \mathcal{L}_A . So, let T_k be the k -th order principal submatrix, which consists of the first k columns and k rows of \mathcal{L}_A , and $t_k = \det(T_k)$, $k = 1, 2, \dots, 3n$. Thus, we can get $t_1 = \frac{2}{3}, t_2 = \frac{1}{3}, t_3 = \frac{2}{15}$, and for $1 \leq i \leq n - 1$,

$$\begin{cases} t_{3i+1} = \frac{4}{5}t_{3i} - \frac{4}{25}t_{3i-1}; \\ t_{3i+2} = t_{3i+1} - \frac{1}{5}t_{3i}; \\ t_{3i+3} = \frac{4}{5}t_{3i+2} - \frac{1}{5}t_{3i+1}. \end{cases}$$

The solution of the previous recurrence relation is

$$\begin{cases} t_{3i-2} = \frac{25}{3} \cdot \left(\frac{2}{25}\right)^i; \\ t_{3i-1} = \frac{25}{6} \cdot \left(\frac{2}{25}\right)^i; \\ t_{3i} = \frac{5}{3} \cdot \left(\frac{2}{25}\right)^i; \end{cases}$$

where $1 \leq i \leq n$.

Now, let S_k be the k -th order principal submatrix, which consists of the last k columns and k rows of \mathcal{L}_A , and $s_k = \det(S_k)$, $k = 1, 2, \dots, 3n$. Thus, we can get $s_1 = \frac{2}{3}, s_2 = \frac{4}{15}, s_3 = \frac{2}{15}$, and for $1 \leq i \leq n - 1$,

$$\begin{cases} s_{3i+1} = \frac{4}{5}s_{3i} - \frac{1}{5}s_{3i-1}; \\ s_{3i+2} = \frac{4}{5}s_{3i+1} - \frac{4}{25}s_{3i}; \\ s_{3i+3} = s_{3i+2} - \frac{1}{5}s_{3i+1}. \end{cases}$$

The solution of the previous recurrence relation is

$$\begin{cases} s_{3i-2} = \frac{25}{3} \cdot \left(\frac{2}{25}\right)^i; \\ s_{3i-1} = \frac{10}{3} \cdot \left(\frac{2}{25}\right)^i; \\ s_{3i} = \frac{5}{3} \cdot \left(\frac{2}{25}\right)^i; \end{cases}$$

where $1 \leq i \leq n$.

Without loss of generality, let $t_0 = 1$ and $s_0 = 1$.

Fact 1. $(-1)^{3n}b_{3n} = \frac{5}{9}(14n + 1)\left(\frac{2}{25}\right)^n$.

$$\begin{aligned}
& + \sum_{0 \leq p \leq q \leq n-1} \det \mathcal{L}_A[3p+1, 3q+2] t_{3p} s_{3n-3q-1} \\
& = \frac{70n^3 + 31n^2 + 37n}{90} \left(\frac{2}{25}\right)^{n-1},
\end{aligned}$$

$$\begin{aligned}
X_3 & = \sum_{0 \leq p < q \leq n} \det \mathcal{L}_A[3p+2, 3q] t_{3p+1} s_{3n-3q+1} + \sum_{0 \leq p < q \leq n} \det \mathcal{L}_A[3p+2, 3q+1] t_{3p+1} s_{3n-3q} \\
& + \sum_{0 \leq p < q \leq n-1} \det \mathcal{L}_A[3p+2, 3q+2] t_{3p+1} s_{3n-3q-1} \\
& = \frac{2}{45} (14n^3 + 9n^2 - n) \left(\frac{2}{25}\right)^{n-1}.
\end{aligned}$$

Thus, we can obtain

$$(-1)^{3n-1} b_{3n-1} = X_1 + X_2 + X_3 = \frac{98n^3 + 21n^2 + 9n}{45} \left(\frac{2}{25}\right)^{n-1},$$

which is the desired result. ■

Together with (4.3) and Facts 1 - 2, one can get the following lemma.

Lemma 4.1. Assume that $0 = \gamma_1 < \gamma_2 \leq \gamma_3 \leq \dots \leq \gamma_{3n+1}$ are the eigenvalues of \mathcal{L}_A , then one gets

$$\sum_{i=2}^{3n+1} \frac{1}{\gamma_i} = \frac{98n^3 + 21n^2 + 9n}{28n + 2}.$$

According to (4.1) - (4.2) and Lemma 4.1, we obtain the following theorem.

Theorem 4.2. For linear crossed phenylenes C_n , we have

$$Kf^*(C_n) = \frac{294n^3 + 287n^2 + 99n + 4}{3}.$$

The multiplicative degree-Kirchhoff indices of C_n are shown in Table 2, where $1 \leq n \leq 15$.

Table 2. Multiplicative degree-Kirchhoff indices from C_1 to C_{15} .

G	$Kf^*(G)$	G	$Kf^*(G)$	G	$Kf^*(G)$	G	$Kf^*(G)$	G	$Kf^*(G)$
C_1	208.00	C_4	7688.00	C_7	37806.00	C_{10}	106438.00	C_{13}	229460.00
C_2	1166.00	C_5	14428.00	C_8	55620.00	C_{11}	140618.00	C_{14}	285298.00
C_3	3463.33	C_6	24271.33	C_9	78301.33	C_{12}	181429.33	C_{15}	349531.33

Theorem 4.3. Assume that C_n are the linear crossed phenylenes, then

$$\lim_{n \rightarrow \infty} \frac{Kf^*(C_n)}{Gut(C_n)} = \frac{1}{4}.$$

Proof. By first classifying and discussing the following cases of vertices, the Gutman index of C_n is obtained.

- Vertex $3i - 1$ ($i = 1, 2, \dots, n$) of C_n :

$$\begin{aligned}
 g_{3i-1} &= 2 \sum_{i=1}^n [4 \times 4 \times 2 + 2 \times 3 \times 4 \times (3i - 2) + 2 \times 3 \times 4 \times (3n - 3i + 2) \\
 &\quad + 2 \sum_{k=1}^{i-1} 4 \times 4 \times 3 \times (i - k) + 2 \sum_{k=i+1}^n 4 \times 4 \times 3 \times (k - i) \\
 &\quad + 2 \sum_{k=2}^i 4 \times 5 \times (3i - 3k + 1) + 2 \sum_{k=i+1}^n 4 \times 5 \times (3k - 3i - 1) \\
 &\quad + 2 \sum_{k=1}^{i-1} 4 \times 5 \times (3i - k - 1) + 2 \sum_{k=i}^n 4 \times 5 \times (3k - 3i + 1)] \\
 &= 8(28n^3 + 3n^2 + 5n).
 \end{aligned}$$

- Vertex $3i$ ($i = 1, 2, \dots, n$) of C_n :

$$\begin{aligned}
 g_{3i} &= 2 \sum_{i=1}^n [5 \times 5 \times 1 + 2 \times 3 \times 5 \times (3i - 1) + 2 \times 3 \times 5 \times (3n - 3i + 1) \\
 &\quad + 2 \sum_{k=1}^i 4 \times 5 \times (3i - 3k + 1) + 2 \sum_{k=i+1}^n 4 \times 5 \times (3k - 3i - 1) \\
 &\quad + 2 \sum_{k=2}^i 5 \times 5 \times (3i - 3k + 2) + 2 \sum_{k=i+1}^n 5 \times 5 \times (3k - 3i - 2) \\
 &\quad + 2 \sum_{k=1}^{i-1} 5 \times 5 \times 3 \times (i - k) + 2 \sum_{k=i+1}^n 5 \times 5 \times 3 \times (k - i)] \\
 &= 10(28n^3 + 3n^2).
 \end{aligned}$$

- Vertex $3i - 2$ ($i = 2, 3, \dots, n$) of C_n :

$$\begin{aligned}
 g_{3i-2} &= 2 \sum_{i=2}^n [5 \times 5 \times 1 + 2 \times 3 \times 5 \times (3i - 3) + 2 \times 3 \times 5 \times (3n - 3i + 3) \\
 &\quad + 2 \sum_{k=1}^{i-1} 4 \times 5 \times (3i - 3k - 1) + 2 \sum_{k=i}^n 4 \times 5 \times (3k - 3i + 1) \\
 &\quad + 2 \sum_{k=2}^{i-1} 5 \times 5 \times 3 \times (i - k) + 2 \sum_{k=i+1}^n 5 \times 5 \times 3 \times (k - i) \\
 &\quad + 2 \sum_{k=1}^{i-1} 5 \times 5 \times (3i - 3k - 2) + 2 \sum_{k=i}^n 5 \times 5 \times (3k - 3i + 2)] \\
 &= 10(28n^3 - 39n^2 + 16n - 5).
 \end{aligned}$$

• Corner vertex of C_n :

$$\begin{aligned}
 g_o &= 2[3 \times 3 \times 1 + 2 \times 3 \times 3 \times 3n + 2(\sum_{i=1}^n 3 \times 4(3i - 2) \\
 &\quad + \sum_{i=1}^n 3 \times 5 \times (3i - 1) + \sum_{i=2}^n 3 \times 5 \times (3i - 3))] \\
 &\quad + 2[3 \times 3 \times 1 + 2 \times 3 \times 3 \times 3n + 2(\sum_{i=1}^n 3 \times 4 \times (3n - 3i + 2) \\
 &\quad + \sum_{i=1}^n 3 \times 5 \times (3n - 3i + 1) + \sum_{i=2}^n 3 \times 5 \times (3n - 3i + 3))] \\
 &= 504n^2 + 36n + 36.
 \end{aligned}$$

Applying (1.4), we obtain

$$Gut(C_n) = \frac{g_o + g_{3i-1} + g_{3i-2} + g_{3i}}{2} = 392n^3 + 84n^2 + 118n - 7.$$

Combining with $Kf^*(C_n)$ and $Gut(C_n)$, one has

$$\lim_{n \rightarrow \infty} \frac{Kf^*(C_n)}{Gut(C_n)} = \frac{1}{4}.$$

This completes the proof. ■

In the following, we can calculate the complexity of C_n .

Theorem 4.4. *For linear crossed phenylenes C_n , we have*

$$\tau(C_n) = 2^{7n+2} \cdot 3^{2n-1}.$$

Proof. Based on Theorem 2.2, we can get $\prod_{i=1}^{6n+2} d_i \prod_{i=2}^{3n+1} \gamma_i \prod_{i=1}^{3n+1} \delta_i = 2(14n + 1)\tau(C_n)$, where

$$\prod_{i=1}^{6n+2} d_i = 3^4 \cdot 4^{2n} \cdot 5^{4n-2},$$

$$\prod_{i=2}^{3n+1} \gamma_i = (-1)^{3n} b_{3n} = \frac{5}{9} \cdot (14n + 1) \cdot \left(\frac{2}{25}\right)^n,$$

$$\prod_{i=1}^{3n+1} \delta_i = \left(\frac{4}{3}\right)^2 \cdot \left(\frac{6}{5}\right)^{2n-1}.$$

Hence,

$$\tau(C_n) = 2^{7n+2} \cdot 3^{2n-1}.$$

The result is as desired. ■

The complexity of C_n is shown in Table 3, where $1 \leq n \leq 12$.

Table 3. The complexity from C_1 to C_{12} .

G	$\tau(G)$	G	$\tau(G)$
C_1	1536	C_7	3590096234354105647104
C_2	1769472	C_8	4135790861975929705463808
C_3	2038431744	C_9	4764431072996271020694306816
C_4	2348273369088	C_{10}	5488624596091704215839841452032
C_5	2705210921189376	C_{11}	6322895534697643256647497352740864
C_6	3116402981210161152	C_{12}	7283975655971685031657916950357475328

5. Conclusions

Based on the Laplacian (normalized Laplacian, resp) polynomial of C_n , we determined the Kirchhoff index, multiplicative degree-Kirchhoff index, and complexity of linear crossed phenylenes through the decomposition theorem and Vieta's Theorem. In addition, we found that the Kirchhoff index and multiplicative degree-Kirchhoff index of linear crossed phenylenes were approximately one quarter of their Wiener index and Gutman index, respectively, which further enriched the results of the Kirchhoff index, multiplicative degree-Kirchhoff index, and complexity for the linear crossed chains.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

All authors declare no conflicts of interest in this paper.

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