Hindawi
Journal of Chemistry
Volume 2019, Article ID 6073905, 7 pages
https://doi.org/10.1155/2019/6073905

Research Article

The Exact Controllability of the Molecular Graph Networks

Liang Wei[1,2] **Faxu Li**[3] **Haixing Zhao**[3] **Bo Deng,**[2] **and Zhonglin Ye**[3]

[1]*School of Computer Science, Shaanxi Normal University, Xi'an 710062, China*
[2]*School of Mathematics and Statistics, Qinghai Normal University, Xining 810008, China*
[3]*College of Computer, Qinghai Normal University, Xining 810008, China*

Correspondence should be addressed to Faxu Li; lifaxu@qhnu.edu.cn

Received 30 July 2019; Accepted 18 October 2019; Published 30 November 2019

Guest Editor: Jia-Bao Liu

In this paper, we mainly study the exact controllability of several types of extended-path molecular graph networks. Based on the construction of extended-path molecular graph networks with C_3, C_4, or K_4, using the determinant operation of the matrix and the recursive method, the exact characteristic polynomial of these networks is deduced. According to the definition of minimum driver node number N_D, the exact controllability of these networks is obtained. Moreover, we give the minimum driver node sets of partial small networks.

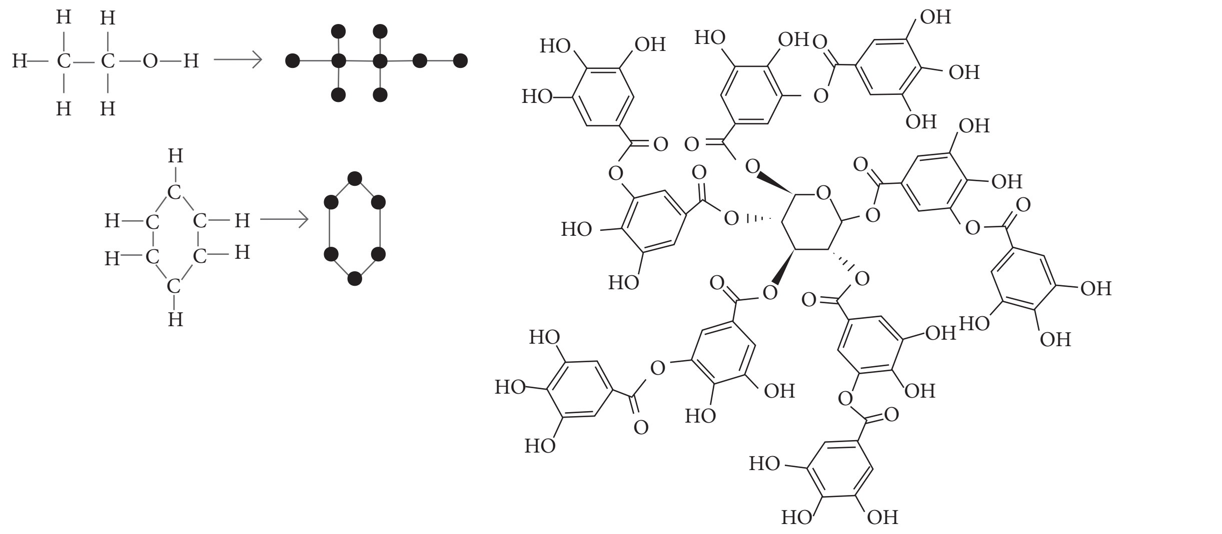
1. Introduction

In recent years, the research on complex network is one of the hottest research fields, and controllability of complex network is a challenging problem in modern network science, such as molecular graph networks, computer networks, social networks, biological networks, and transportation networks [1–8]. The study of network structure has always been a basic object in complex network research. The majority of core issues of research in many fields are based on the structure of the networks, such as connectivity, robustness, and controllability of networks.

In chemical graph theory, the vertices represent each atom and the edges represent the bonds between them in the molecule, and the corresponding molecular graph represents different chemical structures when they represent different things. Figure 1(a) shows the representation of two small molecular structures. As the molecular scale increases, the molecular graph structure gradually becomes a complex system, an example as shown in Figure 1(b). Generally, researchers investigate the related problems of complex systems with large molecular structure by using methods of studying complex networks. In addition, molecular graphs can be used to express some topological properties of molecules. The topological properties of molecules with the same connected structure should be identical. The quantity describing the topological properties of molecules is topological invariants of molecular graphs, such as number of nodes, number of edges, shortest distance, and spectrum. In order to quantify the topological properties of molecules, researchers proposed a lot of indexes, such as Wiener index, Randic index, Hosoya index, Merrifield–Simmons index, and molecular information index.

With the development of network science, people begin to pay much attention to study how to control some nodes in the network to achieve the desirable goals, namely, making the network controllable. The structural controllability of molecular graphs is studied as a molecular topological index. Lin firstly gives the concept of structural controllability in the literature [9] and presents the structural controllability theorem. In the literature [10], the structural controllability theorem is applied to the directed and unweighted complex networks, and the maximum matching theory and the minimum input theorem of structural controllability are proposed.

However, when the edges of the networks are undirected or weighted, the previous theory is not suitable for this type of networks. Then, researchers present another theory framework, which is the exact controllability analysis of the complex network. Yuan et al. [11] proves



(a) (b)

Figure 1: Transformation from molecular structure to molecular graph network. Representation of (a) two small molecular structures and (b) a large molecular structure.

that the number of driver nodes of a network is equal to the maximum geometric multiplicity and gives a method to solve the minimum set of driver nodes. In [12], Wu et al. constructs a star-type network and gives its characteristic polynomial, which directly expresses the exact controllability of this kind of complex networks. Furthermore, research on controllability of multilayer networks and fractal networks, which is common in the chemical system, has some results [13, 14].

In chemistry, hexagonal chain and polyomino chain are two kinds of classical linear systems. In order to observe different linear systems, we consider the controllability of complex networks with linear dynamics. A network with N nodes is described by the following set of ordinary differential equations [15]:

$$\dot{x} = A\mathbf{x} + B\mathbf{u}, \tag{1}$$

where $\mathbf{x} = (x_1, x_2, x_3 \ldots, x_N)^T$ is the status of nodes, $A \in R^{N\times N}$ denotes the coupling matrix of the system, in which a_{ij} represents the weight of a link (i, j) and $\mathbf{u} = (u_1, u_2, u_3 \ldots, u_M)^T$ is the status of M controllers, and B is the control matrix with the size of $N \times M$. In classic control theory, the system (1) can be controlled from any initial state to any final state with finite time if and only if

$$\operatorname{rank}\left(\left[B, AB, A^2B, \ldots, A^{N-1}B\right]\right) = N. \tag{2}$$

Generally, solving the controllability problems is to construct a suitable control matrix B, which consists of a minimum set of driver nodes for satisfying the Kalman rank condition [16]. And there are many possible control matrices B for system (1), which satisfies the controllable condition. The main task of exact controllability is to find a set of B corresponding to the minimum number N_{D} of controllers, which can control the whole network. Then, it is important to measure the exact controllability of the system (1). For undirected graphs, the system controllability can be given by the following terms:

$$N_{\mathrm{D}} = \max_i\{\delta(\lambda_i)\}, \tag{3}$$

where $\delta(\lambda_i)$ is the algebraic multiplicity of eigenvalue of matrix A. It is well known that the theory of graph spectra is related to the chemistry through the HMO (Huckel Molecular Orbital) theory [1]. At an early stage, it was supposed that HMO theory could be reduced to the study of graph spectra of the adjacency matrix of molecular graphs.

In subsequent sections, we mainly discuss the undirected graph with link unweight. Firstly, we give some construction methods of the extended-path molecular graph networks. By using the controllability theory in Sections 3 and 4, we then analyze the exact controllability of these networks and characterize all minimum sets of driver nodes of partial small networks by simulation.

2. Construction of the Extended-Path Networks

In real world, we can find a class of regular networks [17–19], which is constructed like a path network, and each component looks like a star, circle, or clique. In order to carry out our research, we must construct some networks with such characteristics.

Firstly, we give the construction method of the *H*-extended-path networks (*H-EPN*), which is composed of several subgraphs pasted together by one common node. As shown in Figure 2(b), *H-EPN* is composed of subgraph H, the number of H is N, and it satisfies that every two subgraph are connected by one common node. In other words, each edge of the path (Figure 2(a)) can be extended by a subgraph H, which can be connected to each other at a common node. We likewise construct several types of *H-EPNs* as shown in Figures 3(a)–3(d).

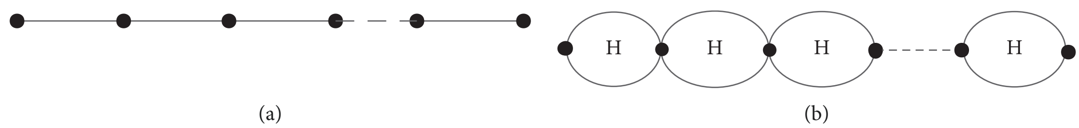


FIGURE 2: Construction of extended-path networks. (a) Path networks. (b) Extended-path networks.

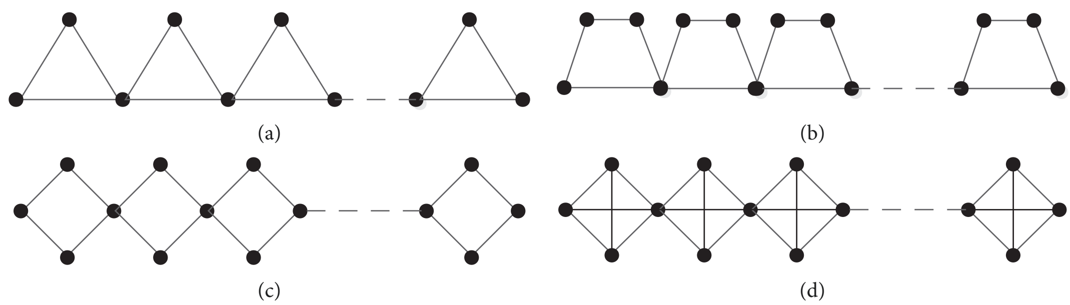


FIGURE 3: *H-EPN* extended by C_3, C_4, and K_4. (a) C_3-*EPN*. (b) C_4-*EPN*1. (c) C_4-*EPN*2. (d) K_4-*EPN*.

3. Main Results

In this section, we will study the exact controllability of several extended-path networks, which are extended by C_3, C_4, and K_4.

The adjacent matrix of C_3-*EPN* can be formalized as follows:

$$A = \begin{bmatrix} 0 & 1 & 1 & & & \\ 1 & 0 & 1 & & & \\ 1 & 1 & 0 & 1 & 1 & \\ & & 1 & 0 & 1 & \\ & & 1 & 1 & 0 & \\ & & & & & \cdots \end{bmatrix}. \quad (4)$$

Therefore, we can obtain the characteristic polynomial of the coupling matrix A of C_3-*EPN* with $2N+1$ nodes. For convenience, we use B_{2N+1} to represent the determinant of matrix $\lambda I - A$ as follows:

$$|\lambda I - A| = B_{2N+1} = \begin{vmatrix} \lambda & -1 & -1 & & & \\ -1 & \lambda & -1 & & & \\ -1 & -1 & \lambda & -1 & -1 & \\ & & -1 & \lambda & -1 & \\ & & -1 & -1 & \lambda & \\ & & & & & \cdots \end{vmatrix} = \left(\lambda^2 - 1\right) B_{2N-1} - 2(\lambda+1) C_{2N-2}, \quad (5)$$

where

$$C_{2N-2} = \begin{vmatrix} \lambda & -1 & & & \\ -1 & \lambda & -1 & -1 & \\ & -1 & \lambda & -1 & \\ & -1 & -1 & \lambda & \\ & & & & \cdots \end{vmatrix}. \quad (6)$$

Thus, it follows that

$$B_{2N+1} = \left(\lambda^2 - 1\right) B_{2N-1} - 2(\lambda+1) C_{2N-2}, \quad (7)$$

$$C_{2N-2} = \lambda B_{2N-3} + \lambda C_{2N-4}. \quad (8)$$

According to the equations (7) and (8), we have

$$B_{2N+1} - \left(\lambda^2 + \lambda - 1\right) B_{2N-1} + \left(\lambda^3 + 2\lambda^2 + \lambda\right) B_{2N-3} = 0. \quad (9)$$

For convenience of calculation, take $S_N = B_{2N+1}$. Then,

$$\begin{aligned} S_{N-1} &= B_{2N-1}, \\ S_{N-2} &= B_{2N-3}. \end{aligned} \quad (10)$$

So we have

$$S_N - \left(\lambda^2 + \lambda - 1\right) S_{N-1} + \left(\lambda^3 + 2\lambda^2 + \lambda\right) S_{N-2} = 0. \quad (11)$$

According to the recursive method in the theory of the determinant, the characteristic equation of recursive relations [11] is given by

$$m^2 - \left(\lambda^2 + \lambda - 1\right) m + \left(\lambda^3 + 2\lambda^2 + \lambda\right) = 0. \quad (12)$$

It is easy to get

$$\begin{aligned} m_1 &= \frac{\left(\lambda^2 + \lambda - 1\right) + p}{2}, \\ m_2 &= \frac{\left(\lambda^2 + \lambda - 1\right) - p}{2}, \end{aligned} \quad (13)$$

where $p = \sqrt{\lambda^4 - 2\lambda^3 - 9\lambda^2 - 6\lambda + 1}$.

Thus, we give the form of solution of S_N in the following expression:

$$S_N = k_1 m_1^N + k_2 m_2^N. \quad (14)$$

For $S_0 = B_1 = \lambda$ and $S_1 = B_3 = \lambda^3 - 3\lambda - 2$, we have $k_1 + k_2 = \lambda$ and $k_1 m_1 + k_2 m_2 = \lambda^3 - 3\lambda - 2$.

So we get

$$k_1=\frac{\lambda^3-3\lambda-2-\lambda m_2}{m_1-m_2}=\frac{1}{p}\left(\lambda^3-3\lambda-2-\lambda m_2\right),$$
$$k_2=\frac{\lambda^3-3\lambda-2-\lambda m_1}{m_1-m_2}=\frac{1}{p}\left(\lambda^3-3\lambda-2-\lambda m_1\right). \tag{15}$$

After an arrangement of equations (13)–(15), we have

$$S_N=k_1m_1^N+k_2m_2^N=\frac{1}{2p}(\lambda+1)^2\Big[(\lambda-2)\left(m_1^N-m_2^N\right)-\lambda^2\left(m_1^{N-1}-m_2^{N-1}\right)\Big]. \tag{16}$$

According to equations (5) and (10), the characteristic polynomial of matrix A is as follows:

$$|\lambda I-A|=B_{2N+1}=S_N=\frac{1}{2p}(\lambda+1)^2\left[(\lambda-2)\left(m_1^N-m_2^N\right)-\lambda^2\left(m_1^{N-1}-m_2^{N-1}\right)\right]. \tag{17}$$

Let $g(\lambda)=(\lambda-2)(m_1^N-m_2^N)-\lambda^2(m_1^{N-1}-m_2^{N-1})$, then it is easy to get that $g(-1)\neq 0$, $g(1)\neq 0$, and $g(0)\neq 0$. So the multiplicity of eigenvalue -1 is 2. Now, we discuss the multiplicity of the remaining eigenvalues. We all know from equations (7) and (9) that if there is an eigenvalue λ_0 making $B_{2N+1}=0$ and suppose that $C_{2N-2}=0$, then it must be $B_{2N-1}=0$ and $B_{2N-3}=0$ (note that 1 and 0 are not roots of the $B_{2N+1}=0$), which is a contradiction with λ_0 being the root of all $B_{2i+1}(\lambda_0)=0$, $(i=1,2,\ldots,N)$.

Now, we show that there is a principal minor determinant of order $2N$ for B_{2N+1} such that the value is not 0 as follows:

$$A'=\begin{vmatrix}\lambda & -1 & & & & & \\ -1 & \lambda & & & & & \\ & & \lambda & -1 & & & \\ & & -1 & \lambda & -1 & -1 & \\ & & & -1 & \lambda & -1 & \\ & & & -1 & -1 & \lambda & \\ & & & & & & \ldots\end{vmatrix}=\begin{vmatrix}\lambda & -1\\ -1 & \lambda\end{vmatrix}C_{2N-2}, \tag{18}$$

which is constructed by deleting the 3th row and the 3th volume of B_{2N+1}. For $C_{2N-2}\neq 0$ and $\begin{vmatrix}\lambda & -1\\ -1 & \lambda\end{vmatrix}\neq 0$ when $\lambda\neq -1$, we have $A'\neq 0$. By $B_{2N+1}=0$ and $A'\neq 0$ in the case of $\lambda\neq -1$, we see that the rank of the corresponding matrix of B_{2N+1} is $2N$. Then, for all the eigenvalues $\lambda\neq -1$, its multiplicity is 1. So we know that all roots of $B_{2N+1}=0$ are distinct except -1.

According to the above analysis, it can be known that the maximum multiplicity of the solution of the equation (17) is 2. Therefore, we get the minimum number of driver nodes in the C_3-EPN as follows:

$$N_{\mathrm{D}}=2. \tag{19}$$

Using the same way, we investigate the exact controllability of the C_4-$EPN1$. The adjacent matrix A of the C_4-$EPN1$ can be formalized as follows:

$$A=\begin{bmatrix}0&1&0&1&&&&\\1&0&1&0&&&&\\0&1&0&1&&&&\\1&0&1&0&1&0&1&\\&&&1&0&1&0&\\&&&0&1&0&1&\\&&&1&0&1&0&\\&&&&&&&\ldots\end{bmatrix}. \tag{20}$$

We obtain the characteristic polynomial of the matrix A as follows:

$$|\lambda I-A|=\begin{vmatrix}\lambda&-1&0&-1&&&&\\-1&\lambda&-1&0&&&&\\0&-1&\lambda&-1&&&&\\-1&0&-1&\lambda&-1&0&-1&\\&&&-1&\lambda&-1&0&\\&&&0&-1&\lambda&-1&\\&&&-1&0&-1&\lambda&\\&&&&&&&\ldots\end{vmatrix}. \tag{21}$$

Let $B_{3N+1}=|\lambda I-A|$, and taking a series of determinant operations, one gets the form as follows:

$$B_{3N+1}=|\lambda I-A|=\lambda^2C_{3N-1}-2\lambda B_{3N-2}, \tag{22}$$

$$C_{3N-1}=\lambda B_{3N-2}-2D_{3N-3}, \tag{23}$$

$$D_{3N-3}=\left(\lambda^2-1\right)B_{3N-5}-\lambda D_{3N-6}, \tag{24}$$

where C_{3N-1} and D_{3N-3} are determinants with the size of $(3N-1)\times(3N-1)$ and $(3N-3)\times(3N-3)$, respectively. We can formalise them as follows:

$$C_{3N-1}=\begin{vmatrix}\lambda&-1&&&&&\\-2&\lambda&-1&0&-1&&\\&-1&\lambda&-1&0&&\\&0&-1&\lambda&-1&&\\&-1&0&-1&\lambda&&\\&&&&&&\ldots\end{vmatrix},$$
$$D_{3N-3}=\begin{vmatrix}\lambda&-1&0&&&&\\-1&\lambda&-1&&&&\\0&-1&\lambda&-1&0&-1&\\&&-1&\lambda&-1&0&\\&&0&-1&\lambda&-1&\\&&-1&0&-1&\lambda&\\&&&&&&\ldots\end{vmatrix}. \tag{25}$$

Through the equations (22)–(24), we get the following form of recurrence relationship:

$$B_{3N+1} = \left(\lambda^3 - 3\lambda\right) B_{3N-2} - \lambda^4 B_{3N-5}. \quad (26)$$

Now, let us define $S_N = B_{3N+1}, S_{N-1} = B_{3N-2}$, and $S_{N-2} = B_{3N-5}$, then the equation (26) can be formalized as

$$S_N = \left(\lambda^3 - 3\lambda\right) S_{N-1} - \lambda^4 S_{N-2}. \quad (27)$$

According to the above definitions and equation (27), we have $S_0 = B_1 = \lambda$ and $S_1 = B_4 = \lambda^2(\lambda^2 - 4)$, so

$$S_2 = \left(\lambda^3 - 3\lambda\right) S_1 - \lambda^4 S_0 = \lambda^3\left(\lambda^4 - 8\lambda^2 + 12\right) = \lambda^3 f_2(\lambda), \quad (28)$$

where $f_i(x)$ represents the i-th polynomial about x, for which the lowest order is 0. Fox example, $f_0(\lambda) = 1$, $f_1(\lambda) = \lambda^2 - 4$, and $f_2(\lambda) = \lambda^4 - 8\lambda^2 + 12$. Obviously, we can get remaining items formalized as

$$\begin{aligned} S_3 &= \left(\lambda^3 - 3\lambda\right) S_2 - \lambda^4 S_1 = \lambda^4 f_3(\lambda), \\ S_4 &= \left(\lambda^3 - 3\lambda\right) S_3 - \lambda^4 S_2 = \lambda^5 f_4(\lambda), \\ &\ldots \\ S_N &= \left(\lambda^3 - 3\lambda\right) S_{N-1} - \lambda^4 S_{N-2} = \lambda^{N+1} f_N(\lambda). \end{aligned} \quad (29)$$

Using a simple induction and computation, we can easily get (29). That is to say, the lowest orders of polynomials S_0, $S_1, S_2, \ldots$, and S_N are $1, 2, 3, \ldots$, and $N + 1$, respectively, and the multiplicity of the eigenvalue 0 of S_N is $N + 1$. Since a connected graph with diameter D has at least $D + 1$ distinct eigenvalues, noticing that the network C_4-$EPN1$ with N cells has $3N + 1$ nodes and the diameter is $N + 2$, we have that C_4-$EPN1$ has at least $N + 3$ distinct eigenvalues. However, the eigenvalue 0 has a multiplicity of $N + 1$, and the remaining $2N$ eigenvalues have at least $N + 2$ distinct, namely, the maximum multiplicity of these eigenvalues shall not exceed $N - 1$. Therefore, the maximum multiplicity of C_4-$EPN1$'s eigenvalues is $N + 1$ (the eigenvalue is 0). Thus, the minimum number of driver nodes of the system corresponding to the graph C_4-$EPN1$ is as follows:

$$N_D = N + 1. \quad (30)$$

By the analytical method of the preceding part, we can obtain the recursive relations of characteristic polynomial of C_4-$EPN2$ and K_4-EPN (see (31) and (32)) as follows:

$$S_N = \left(\lambda^3 - 4\lambda\right) S_{N-1} - \lambda^4 S_{N-2} = \lambda^{N+1} f_N(\lambda), \quad (31)$$

$$\begin{aligned} S_N &= (\lambda + 1)\left(\lambda^2 - \lambda - 4\right) S_{N-1} - (\lambda + 1)^4 S_{N-2} \\ &= (\lambda + 1)^{N+2} f_N(\lambda + 1). \end{aligned} \quad (32)$$

Using a method similar to that of the C_3-EPN and C_4-$EPN1$, it is easy to get that the minimum number of driver nodes of C_4-$EPN2$ and K_4-EPN, shown in Table 1.

4. Characterization of Driver Nodes

The topology of the complex network determines the controllability, and the minimum driver nodes can quantitatively reflect the controllability of the network structures. Therefore, the minimum driver nodes are the key factors in the structural controllability analysis. In fact, evaluating the exact controllability of complex networks is to obtain the minimum driver nodes of networks.

Using the method based on the PBH rank criterion [11, 20], we can characterize the minimum driver node set in detail. The condition of the full rank of the matrix $[\lambda I - A \;\; B]$ is

(1) Matrix $\lambda I - A$ avoids zero vector

(2) Matrix $\lambda I - A$ avoids repetitive vector

(3) Matrix $\lambda I - A$ avoids correlation vector

Because of the symmetry of graph structures, the minimum driver nodes set is not unique and its number is mainly determined by three factors such as zero row vector, repetitive row vector, and correlation row vector of $[\lambda I - A]$.

Let zero vector have x rows, repetitive row vector have y groups, in which each group has $r_1, r_2, \ldots, r_y$ rows, and the correlation row vectors have z groups, in which each group has $c_1, c_2, \ldots, c_z$ rows; then, the number of the minimum driver nodes N_D and the number of groups obtained N_C are shown in Table 2.

Based on the above conditions, we design a corresponding algorithm to obtain the minimum driver nodes set. Through simulation analysis of Matlab platform, we compute the controllability, and describe all sets of minimal driver nodes of C_3-EPN, C_4-EPN, and K_4-EPN(N=4, 5), respectively; they are shown in Tables 3, 4 and 5; H-EPNs of $N = 4$ are shown in Figure 4.

The simulation results show that, in order to fully control these extended-path networks, the driver nodes selected are usually nodes with small degree, rather than the maximum degree nodes. The point is consistent with the conclusion in the literature [11]. And we can obtain from Table 3 that the C_3-EPN has a fixed number of minimum driver node set, which can be fully controlled by minimal cost. Namely, the C_3-EPN has higher controllability. In addition, although the structures of the C_4-$EPN1$ and C_4-$EPN2$ are different, we find that the controllability of the two networks is exactly the same in different network scales.

Table 1: N_D of extended-path networks.

Networks	Number of cells	n	N_D
C_3-EPN	N	$2N + 1$	2
C_4-$EPN1$	N	$3N + 1$	$N + 1$
C_4-$EPN2$	N	$3N + 1$	$N + 1$
K_4-EPN	N	$3N + 1$	$N + 2$

Table 2: N_D and N_C of three kinds of situations.

Case	N_D	N_C
Zero row vector	x	1
Repetitive row vector	$\sum_{i=1}^{y}(r_i - 1)$	$\prod_{i=1}^{y}(C_{r_i}^{r_i-1})$
Correlation row vector	z	$\prod_{j=1}^{z}(C_{c_j}^{1})$

Table 3: Controllability of C_3-*EPN*, C_4-*EPN*, and K_4-*EPN* ($N = 4$, 5).

Networks	Number of cell (N)	Number of nodes (n)	Minimum driver node (N_D)	Controllability (N_D/n)
C_3-*EPN*	4	9	2	0.2222
C_4-*EPN*1	4	13	5	0.3846
C_4-*EPN*2	4	13	5	0.3846
K_4-*EPN*	4	13	6	0.4615
C_3-*EPN*	5	11	2	0.1818
C_4-*EPN*1	5	16	6	0.3750
C_4-*EPN*2	5	16	6	0.3750
K_4-*EPN*	5	16	7	0.4375

Table 4: Minimum driver nodes set of C_3-*EPN*, C_4-*EPN*, and K_4-*EPN* ($N = 4$).

Networks	Minimum driver node set
C_3-*EPN*	$\{(n1, n2) \mid n1 \in \{1,2\}, n2 \in \{8,9\}\}$
C_4-*EPN*1	$\{(1, n1, n2, n3, n4) \mid n1 \in \{2,3\}, n2 \in \{5,6\}, n3 \in \{8,9\}, n4 \in \{11,12\}\}$, or $\{(n1, n2, n3, n4, 13) \mid n1 \in \{2,3\}, n2 \in \{5,6\}, n3 \in \{8,9\}, n4 \in \{11,12\}\}$
C_4-*EPN*2	$\{(n1, 10, 11, 12, 13) \mid n1 \in \{1,3\}\}$, or $\{(1,2,3,4,n1) \mid n1 \in \{11,13\}\}$
K_4-*EPN*	$\{(n1, n2, n3, n4, n5, n6) \mid n1 \in \{1,2,3\}, n2 \in \{1,2,3\}, n1 \neq n2, n3 \in \{5,6\}, n4 \in \{8,9\}, n5 \in \{11,12,13\}, n6 \in \{11,12,13\}, n5 \neq n6\}$

Table 5: Minimum driver node set of C_3-*EPN*, C_4-*EPN*, and K_4-*EPN* ($N = 5$).

Networks	Minimum driver node set
C_3-*EPN*	$\{(n1, n2) \mid n1 \in \{1,2\}, n2 \in \{10,11\}\}$
C_4-*EPN*1	$\{(1, n1, n2, n3, n4, n5) \mid n1 \in \{2,3\}, n2 \in \{5,6\}, n3 \in \{8,9\}, n4 \in \{11,12\}, n5 \in \{14,15\}\}, n3 \in \{8,9\}, n4 \in \{11,12\}, n5 \in \{14,15\}\}$
C_4-*EPN*2	$\{(n1, 12, 13, 14, 15, 16) \mid n1 \in \{1,3\}\}$, or $\{(1,2,3,4,5,n1) \mid n2 \in \{14,16\}\}$
K_4-*EPN*	$\{(n1, n2, n3, n4, n5, n6, n7) \mid n1 \in \{1,2,3\}, n2 \in \{1,2,3\}, n1 \neq n2, n3 \in \{5,6\}, n4 \in \{8,9\}, n5 \in \{11,12\}, n6 \in \{14,15,16\}, n7 \in \{14,15,16\}, n6 \neq n7\}$

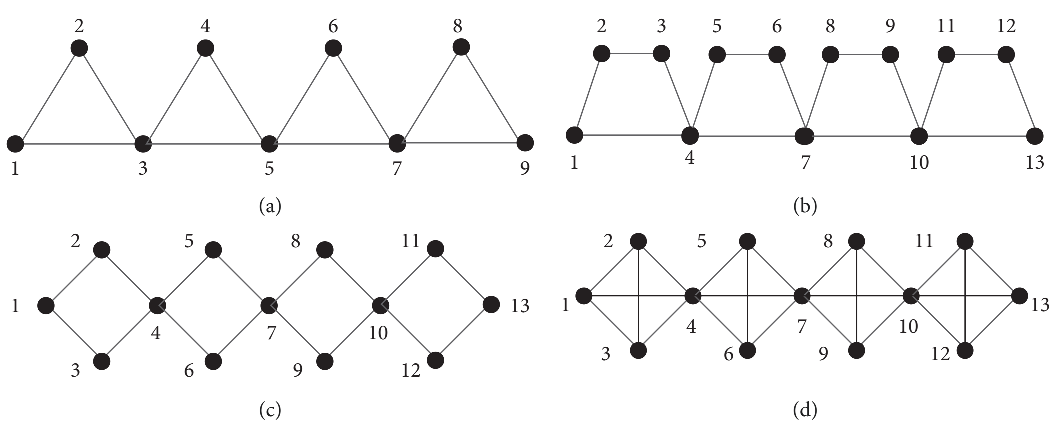


Figure 4: C_3-*EPN*, C_4-*EPN*, and K_4-*EPN* ($N = 4$).

5. Conclusion

To summarize, we mainly study the controllability of several types of the extended-path molecular graph networks. The structural characteristics of these networks are linearly connected by a cycle or complete graph. For these special network structures, we derive the general formula of the characteristic polynomial of the network's adjacent matrix. Furthermore, the exact controllability of these kinds of networks is analyzed, and some results are obtained. In addition, in order to directly reflect the concrete minimum driver node set of each network, we determine the distribution of the nodes by simulation.

Data Availability

All data, models, and codes generated or used during the study are available from the corresponding author upon request.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Acknowledgments

This work was supported by the Nature Science Foundation from Qinghai Province (No. 2018-ZJ-718), the Tibetan Information Processing and Machine Translation Key Laboratory of Qinghai Province, and the Key Laboratory of Tibetan Information Processing, Ministry of Education.

References

[1] A. Graovac, I. Gutman, and N. Trinajstic, *Topological Approach to the Chemistry of Conjugated Molecules*, Springer-Verlag, Berlin, Germany, 1977.

[2] A. Lombardi and M. Hornquist, "Controllability analysis of networks," *Physical Review E*, vol. 75, no. 5, Article ID 056110, 2007.

[3] X. F. Wang and G. R. Chen, "Pinning control of scale-free dynamical networks," *Physica A: Statistical Mechanics and its Applications*, vol. 310, no. 3-4, pp. 521–531, 2002.

[4] B. Liu, T. Chu, L. Wang, and G. Xie, "Controllability of a leader-follower dynamic network with switching topology," *IEEE Transactions on Automatic Control*, vol. 53, no. 4, pp. 1009–1013, 2008.

[5] A. Rahmani, M. Ji, M. Mesbahi, and M. Egerstedt, "Controllability of multi-agent systems from a graph-theoretic perspective," *SIAM Journal on Control and Optimization*, vol. 48, no. 1, pp. 162–186, 2009.

[6] G.-R. Chen, "Problems and challenges in control theory under complex dynamical network environments," *Acta Automatica Sinica*, vol. 39, no. 4, pp. 312–321, 2013.

[7] G. Chen, "Pinning control and synchronization on complex dynamical networks," *International Journal of Control, Automation and Systems*, vol. 12, no. 2, pp. 221–230, 2014.

[8] L. Hou, S. Y. Lao, Y. D. Xiao et al., "Recent progression controllability of complex network," *Acta Physica Sinica*, vol. 64, no. 18, pp. 188901_1–188901_11, 2015, (in Chinese).

[9] C. T. Lin, "Structural controllability," *IEEE Trans Automatic Control*, vol. 19, no. 3, pp. 201–208, 1974.

[10] Y.-Y. Liu, J.-J. Slotine, and A.-L. Barabási, "Controllability of complex networks," *Nature*, vol. 473, no. 7346, pp. 167–173, 2011.

[11] Z. Z. Yuan, C. Zhao, Z. R. Di et al., "Exact controllability of complex networks," *Nature Communications*, vol. 4, no. 1, p. 2447, 2013.

[12] L. P. Wu, J. K. Zhou, Z. Z. Yuan et al., "Exact controllability of a star-type network," in *Proceedings of the 27th Chinese Control and Decision Conference (2015 CCDC)*, Qingdao, China, May 2015, pp. 5187-5191, in Chinese.

[13] Z. Yuan, C. Zhao, W.-X. Wang, Z. Di, and Y.-C. Lai, "Exact controllability of multiplex networks," *New Journal of Physics*, vol. 16, no. 10, Article ID 103036, 2014.

[14] J. Li, Z. Yuan, Y. Fan, W.-X. Wang, and Z. Di, "Controllability of fractal networks: an analytical approach," *EPL (Europhysics Letters)*, vol. 105, no. 5, Article ID 58001, 2014.

[15] J. J. Slotine and W. Li, *Applied Nonlinear Control*, Prentice-Hall, Upper Saddle River, NJ, USA, 1991.

[16] R. E. Kalman, "Mathematical description of linear dynamical systems," *Journal of the Society for Industrial and Applied Mathematics Series A Control*, vol. 1, no. 2, pp. 152–192, 1963.

[17] A. Shafieinejad, F. Hendessi, and F. Fekri, "Star-structure network coding for multiple unicast sessions in wireless mesh networks," *Wireless Personal Communications*, vol. 72, no. 4, pp. 2185–2214, 2013.

[18] A. Jain, A. Vyas, and H. Yadav, "Analysis of ethernet load on various nodes of star network using opnet," *International Journal of Computer Science and Applications (TIJCSA)*, vol. 3, no. 1, 2014.

[19] X. J. Li and J. M. Xu, "Fault-tolerance of (n, k) star network," *Applied Mathematics and Computation*, vol. 248, pp. 525–530, 2014.

[20] X. K. Chen, Y. Lu, and L. Y. Chen, "Network structural controllability analysis based on PBH," *Journal of PLA University of Science and Technology (Natural Science Edition)*.