



# Tutte polynomials for some chemical polycyclic graphs

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Received: 15 April 2023 / Accepted: 3 September 2023

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## Abstract

The Tutte polynomial is a classical polynomial graph invariant that provides important information about the structure of a graph. In this study, we focus on the Tutte polynomials for typical silicate molecular networks and benzenoid systems, and derive exact formulas for the considered polycyclic chemical graphs. We also determine the explicit closed-form analytic expressions for the number of spanning trees, connected spanning subgraphs, spanning forests, and acyclic orientations of these chemical polycyclic graphs. Our approach employs a combinatorial decomposition technique, which is a general method that can be easily extended to other 2-connected chemical polycyclic networks. This research contributes to a better understanding of the topological properties of chemical structures and has potential applications in chemistry and materials science.

**Keywords** Tutte polynomial · Benzenoid system · Silicate network · Spanning tree

## 1 Introduction

Various problems in mathematical chemistry, statistical physics, information sciences, engineering and discrete mathematics can be treated and solved in a rather efficient manner by making use of polynomials. Particularly, graph polynomial has been substantiated to be a powerful tool in the study and analysis of chemical structures represented by graphs in the field of chemical graph theory [1–10]. One of the most useful polynomial invariants in graph theory is the Tutte polynomial. The famous chromatic polynomial, flow polynomial and reliability polynomial can all be deemed as its specializations. The particular evaluations of the Tutte polynomial give several important invariant parameters, such as the number of spanning trees, the number of connected spanning subgraphs, the number of spanning forests, the number of acyclic orientations, and so on. The Tutte polynomial also has a close connection with the

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Abelian sandpile model and the  $q$ -state Potts model in statistical mechanics [11]. Additionally, it can be specialized to the Jones polynomial of an alternating knot or link and the weight enumerator of a linear code over  $GF(q)$ . The zeros and coefficients of the Tutte polynomial have also been a valuable source for investigating various problems in discrete mathematics and related areas. Thus, if the Tutte polynomial of a given network can be obtained, then the advantage is that many relevant graph invariant information can be determined uniformly. Although it is significant to determine the Tutte polynomial of a network completely, obtaining the Tutte polynomial for graphs is generally an outstanding challenge. According to the best of our knowledge and literature, there are only a few well-structured networks whose Tutte polynomials are completely determined. As an important graph structure information carrier, the Tutte polynomials for some individual network models with important application background have also been studied in the past few years [12–16].

As natural graph representations of benzenoid hydrocarbons, hexagonal (benzenoid) systems are of great importance in organic theoretical chemistry [17]. They are defined as finite 2-connected bipartite plane graphs, in which all interior regions are mutually congruent hexagons. Each vertex of a hexagonal system is shared by at most three hexagons. If a vertex belongs to three hexagons in a hexagonal system, then the vertex is called an internal vertex of the corresponding hexagonal system. A hexagonal system is called catacondensed if it does not have internal vertices. Otherwise, it is called pericondensed. Nowadays, there are many research papers devoted to exploring the chemical and mathematical properties of hexagonal systems. In [18, 19], the authors studied the Kekulé number, Fries number, and Clar number for hexagonal systems. The extremal problems of vertex-degree-based topological indices for hexagonal systems are considered in [20]. Lou et al. [21] gave explicit expressions of the characteristic polynomial of a special hexagonal system, and they determined the spectral radius and the multiplicity of eigenvalues  $\pm 1$  of the hexagonal system. Very recently, Ita et al. [22] presented a new method for computing the Merrifield–Simmons index based on some basic graphs. By using transfer matrices, Oz [23] presented a method to compute the number of  $k$ -matchings of arbitrary catacondensed hexagonal systems. For more details on the mathematical chemistry properties of hexagonal systems, we refer to References [10, 24–29].

Silicates, which make up approximately 90% of the earth's crust, are regarded as the largest and most important class of common rock-forming minerals. These minerals are obtained by fusing metal oxides or metal carbonates with sand and are classified based on the structure of their silicate groups. The tetrahedron  $\text{SiO}_4$  is the fundamental unit of silicates, and various silicate molecular networks have been constructed using different arrangements of these tetrahedra. These molecular networks have attracted the attention of scholars worldwide, who have studied their properties extensively. For example, Hayat and Imran [30] investigated the topological indices of certain silicate networks, while Akbari et al. [31, 32] studied the degree-based and distance-based topological indices of silicate networks using vertex cut techniques. Shoaid et al. [33] used electrical network techniques to determine the resistance distance between two arbitrary vertices of linear silicate chains and cyclic silicate networks, as well as the Kirchhoff index of these networks. Recently, Li et al. [34] determined the number of matchings in linear and cyclic silicate molecular graphs. Despite this progress,

the silicate molecular network remains a high-profile molecular structure with many valuable characteristic properties yet to be explored.

Due to the widespread application of the Tutte polynomial, researchers have studied the Tutte polynomial for several chemical polycyclic graphs. For instance, the Tutte polynomials for certain planar polycyclic graphs [35], catacondensed benzenoid systems [12] and phenylene systems with a given number of branching hexagons [36], and pyrene chains and triphenylene chains [37] have been obtained in recent years. However, the Tutte polynomials for silicate networks and some pericondensed benzenoid systems have received a lot of attention lately but remain unstudied. In this paper, we are motivated by the computation results in [33, 34, 38] and continue this topic by computing the Tutte polynomials of some classes of typical silicate molecular networks and pericondensed hexagonal systems. We also show that many structure invariants of such chemical graphs can be expressed as closed-form formulas. The results presented in this paper will be conducive to further understanding the physico-chemical properties of silicate molecular networks and hexagonal systems.

## 2 Preliminaries

Throughout this paper we consider only undirected and connected graphs, and multiple edges and loops are allowable. Let  $G$  be a graph consisting of a finite set  $V(G)$  of vertices and a finite set  $E(G)$  of edges. All terms used but not defined in this paper can be found in [11, 39].

For an undirected graph  $G = (V(G), E(G))$ , the Tutte polynomial can be defined as the following recurrence relation [11]

$$T(G; x, y) = \begin{cases} 1 & \text{if } E(G) = \emptyset, \\ xT(G/e; x, y) & \text{if } e \text{ is a cut edge,} \\ yT(G - e; x, y) & \text{if } e \text{ is a loop,} \\ T(G - e; x, y) + T(G/e; x, y) & \text{otherwise,} \end{cases} \quad (1)$$

where  $G - e$  and  $G/e$  are graphs obtained from  $G$  by deleting and contracting the edge  $e$ , respectively.

If  $G$  is obtained from a graph  $H$  by adding  $b$  cut edges and  $\ell$  loops, then it is clear from (1) that

$$T(G; x, y) = x^b y^\ell T(H; x, y). \quad (2)$$

In terms of the essential characteristic of the Tutte polynomial, some splitting formulas have been established.

**Proposition 2.1** *Let  $G \cdot H$  be the graph obtained from the union of two other graphs  $G$  and  $H$  such that they have only a common vertex. Then*

$$T(G \cdot H; x, y) = T(G; x, y)T(H; x, y). \quad (3)$$

**Proposition 2.2** [40] Let  $G : H$  be the graph obtained from  $G$  and  $H$  such that the intersection of  $V(G)$  and  $V(H)$  has two elements  $\{u, v\}$  and  $E(G) \cap E(H) = \emptyset$ . Then

$$T(G : H; x, y) = \frac{(x-1)T_{G/\{u,v\}}T_{H/\{u,v\}} + (y-1)T_G T_H - T_G T_{H/\{u,v\}} - T_{G/\{u,v\}} T_H}{xy - x - y}, \quad (4)$$

where  $G/\{u, v\}$  denotes the graph obtained from  $G$  by identifying the vertices  $u$  and  $v$  and not need to delete any edges.

It is known that the Tutte polynomial carries rich information about the graphical structure. The following Proposition 2.3 lists partial interesting results.

**Proposition 2.3** [11] Let  $G$  be a connected graph. Then (i)  $T(G; 1, 1)$  is equal to the number of spanning trees  $N_{ST}(G)$ ; (ii)  $T(G; 1, 2)$  is equal to the number of connected spanning subgraphs  $N_{SCS}(G)$ ; (iii)  $T(G; 2, 1)$  is equal to the number of spanning forests  $N_{SF}(G)$ ; (iv)  $T(G; 2, 0)$  is equal to the number of acyclic orientations  $N_{AO}(G)$ .

Let  $N_{ST}(G)$  be the number of spanning trees of graph  $G$ . The asymptotic growth constant of the number of spanning trees  $\kappa(G)$ , also called spanning tree entropy, is an important measure parameter for some topological property of a graph  $G$ , which is defined as

$$\kappa(G) = \lim_{|V(G)| \rightarrow \infty} \frac{\ln N_{ST}(G)}{|V(G)|}. \quad (5)$$

### 3 The Tutte polynomials of silicate networks

In this section, we consider the Tutte polynomials of three classes typical silicate molecular graphs, including the linear silicate chain  $LS_n$ , the cylinder silicate molecular graph  $CS_n$  and the double silicate molecular chain  $DS_n$ , the configurations of  $LS_n$ ,  $CS_n$  and  $DS_n$  are shown respectively in Figs. 1, 2, and 3 for small  $n$ . The basic chemical unit of silicate is a tetrahedron ( $SiO_4$ ) in which the corner vertices represents the oxygen nodes and the central vertex represents the silicon node. These tetrahedra combine in a variety of ways to form molecular networks of silicates. One can observe that the  $SiO_4$  can be represented by the completed graph  $K_4$  in the language of graph theory (see Fig. 1), then it is easy to obtain that

$$T(K_4; x, y) = 3x^2 + x^3 + x(2 + 4y) + y(2 + 3y + y^2)$$

by using the basic formula (1), and we set  $\alpha = \alpha(x, y) = T(K_4; x, y)$  in the ensuing discussion.

#### 3.1 The Tutte polynomial of linear silicate chain $LS_n$

We first give the Tutte polynomial of linear silicate chain  $LS_n$ .

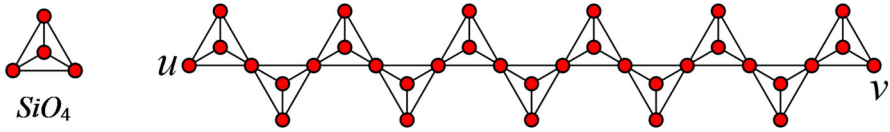


Fig. 1 Tetrahedron (SiO<sub>4</sub>) and the linear silicate molecular chain LS<sub>11</sub>

**Theorem 3.1** *The Tutte polynomial of LS<sub>n</sub> is given by*

$$T(LS_n; x, y) = (3x^2 + x^3 + x(2 + 4y) + y(2 + 3y + y^2))^n.$$

**Proof** Note that  $LS_n = LS_{n-1} \cdot K_4$  and  $LS_1 \cong K_4$ , then one can get that  $T(LS_n, x, y) = T(LS_{n-1}; x, y)T(K_4; x, y)$  by Proposition 2.1. Moreover, we have that  $T(LS_n; x, y) = T(LS_{n-1}; x, y)T(K_4; x, y) = T(LS_{n-2}; x, y)T(K_4; x, y)^2 = \dots = T(LS_1; x, y)T(K_4; x, y)^{n-1} = T(K_4; x, y)^n = \alpha^n = (3x^2 + x^3 + x(2 + 4y) + y(2 + 3y + y^2))^n$ . □

From Theorem 3.1 and Proposition 2.3, the number of spanning trees (spanning connected subgraphs, spanning forests, acyclic orientations) of the linear silicate molecule graph  $LS_n$  can be determined directly.

**Corollary 3.2** *For  $n \geq 1$ , (i) the number of spanning trees of  $LS_n$  is  $N_{ST}(LS_n) = 16^n$ ; (ii) the number of spanning connected subgraphs of  $LS_n$  is  $N_{SCS}(G) = 38^n$ ; (iii) the number of spanning forests of  $LS_n$  is  $N_{SF}(LS_n) = 38^n$ ; (iv) the number of acyclic orientations of  $LS_n$  is  $N_{AO}(LS_n) = 24^n$ .*

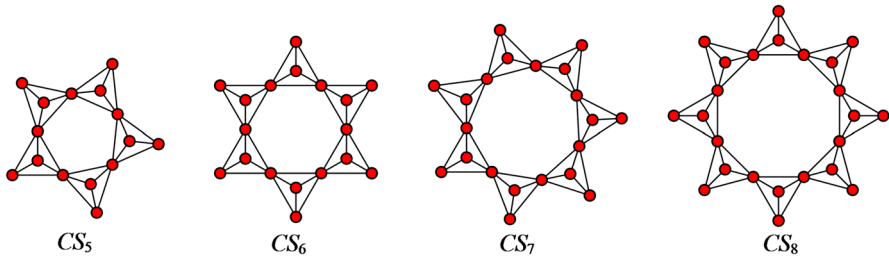
From the structural features of  $LS_n$ , it is easy to get that the linear silicate chain  $LS_n$  consists of  $|V(LS_n)| = 3n + 1$  number of vertices and number of  $|E(LS_n)| = 4n$  edges. Then by (5), the spanning tree entropy of the linear silicate molecular networks can be given by

$$\begin{aligned} \kappa(LS_n) &= \lim_{|V(LS_n)| \rightarrow \infty} \frac{\ln(N_{ST}(LS_n))}{|V(LS_n)|} = \lim_{n \rightarrow \infty} \frac{\ln(16^n)}{3n + 1} = \lim_{n \rightarrow \infty} \frac{n \ln 16}{3n + 1} \\ &= \frac{\ln 16}{3} \approx 0.924196. \end{aligned} \tag{6}$$

### 3.2 The Tutte polynomial of cylinder silicate molecular graph CS<sub>n</sub>

In this subsection, we give the expression of the Tutte polynomial for cylinder silicate molecular graph  $CS_n$ . The cylinder silicate molecular graphs  $CS_5, CS_6, CS_7$  and  $CS_8$  are illustrated in Fig. 2.

**Theorem 3.3** *For  $n \geq 2$ , the Tutte polynomial of  $CS_n$  is  $T(CS_n; x, y) = \phi^{n-2}[(y - 1)\alpha^2 + (x - 1)\beta^2 - 2\alpha\beta](xy - x - y)^{-1} + \psi\alpha^2(\phi^{n-2} - \alpha^{n-2})(\phi - \alpha)^{-1}$ , where  $\alpha = \alpha(x, y) = 3x^2 + x^3 + x(2 + 4y) + y(2 + 3y + y^2)$ ,  $\beta = \beta(x, y) = y(x + y + y^2 + y^3 + (x + y)^2)$ ,  $\phi = \phi(x, y) = 2 + 3x + x^2 + 4y + 2xy + 3y^2 + y^3$  and  $\psi = \psi(x, y) = 2 + 3x + x^2 + 2y$ .*



**Fig. 2** The cylinder silicate molecular graphs  $CS_5$ ,  $CS_6$ ,  $CS_7$  and  $CS_8$

**Proof** Note that the graphs  $CS_n$  and  $CS_{n-1}$  can be constructed respectively by the way of that  $CS_n = LS_{n-1} : K_4$  and  $LS_{n-1}/\{u, v\} = CS_{n-1}$ , where  $u$  and  $v$  are respectively the vertices with degree 3 of the two terminal  $SiO_4$  in  $LS_{n-1}$ . Firstly, from the deletion-contraction formula (1), it is not difficult to get that

$$T(K_4/\{u, v\}) = y(x + y + y^2 + y^3 + (x + y)^2),$$

and, for the sake of convenience, we put  $\beta = \beta(x, y) = T(K_4/\{u, v\})$  in the ensuing discussion. Then one can obtain the following relation by using Proposition 2.2.

$$T(CS_n; x, y) = \frac{(x-1)\beta - \alpha}{xy - x - y} T(CS_{n-1}; x, y) + \frac{\alpha^{n-1}[(y-1)\alpha - \beta]}{xy - x - y}.$$

Setting  $\phi = \phi(x, y) = [(x-1)\beta - \alpha](xy - x - y)^{-1} = 2 + 3x + x^2 + 4y + 2xy + 3y^2 + y^3$  and  $\psi = \psi(x, y) = ((y-1)\alpha - \beta)(xy - x - y)^{-1} = 2 + 3x + x^2 + 2y$ . Thus, from above we have that

$$\begin{aligned} T(CS_n; x, y) &= \phi \cdot T(CS_{n-1}; x, y) + \alpha^{n-1} \cdot \psi \\ &= \phi^2 \cdot T(CS_{n-2}; x, y) + \phi \cdot \alpha^{n-2} \cdot \psi + \alpha^{n-1} \cdot \psi \\ &= \phi^3 \cdot T(CS_{n-3}; x, y) + \phi^2 \cdot \alpha^{n-3} \cdot \psi + \phi \cdot \alpha^{n-2} \cdot \psi + \alpha^{n-1} \cdot \psi \\ &= \dots \\ &= \phi^{n-2} \cdot T(CS_2; x, y) + \psi \sum_{i=2}^{n-1} \alpha^i \phi^{n-1-i} \\ &= \phi^{n-2} \cdot T(CS_2; x, y) + \psi \alpha^2 (\phi^{n-2} - \alpha^{n-2}) (\phi - \alpha)^{-1}. \end{aligned}$$

Moreover, by the use of (4) we can get  $T(CS_2; x, y) = T(K_4 : K_4; x, y) = ((y-1)\alpha^2 + (x-1)\beta^2 - 2\alpha\beta)(xy - x - y)^{-1} = 4x + 12x^2 + 13x^3 + 6x^4 + x^5 + 4y + 20xy + 25x^2y + 10x^3y + x^4y + 12y^2 + 28xy^2 + 16x^2y^2 + 4x^3y^2 + 16y^3 + 22xy^3 + 10x^2y^3 + 15y^4 + 14xy^4 + 2x^2y^4 + 11y^5 + 4xy^5 + 5y^6 + y^7$ . Therefore, the proof is completed.  $\square$

The precise expansion expressions of the Tutte polynomials for the networks  $CS_3$ ,  $CS_4$ ,  $CS_5$ ,  $CS_6$ ,  $CS_7$  and  $CS_8$  are listed in Appendix.

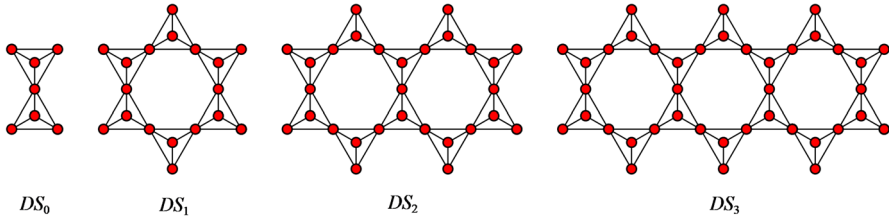


Fig. 3 The double silicate molecular chains  $DS_0$ ,  $DS_1$ ,  $DS_2$  and  $DS_3$

Since it is easy to get that  $\alpha(1, 1) = \phi(1, 1) = 16$ ,  $\beta(1, 1) = \psi(1, 1) = 8$ ,  $\alpha(1, 2) = \phi(1, 2) = 38$ ,  $\beta(1, 2) = 48$ ,  $\psi(1, 2) = 10$ ,  $\alpha(2, 1) = 38$ ,  $\phi(2, 1) = 24$  and  $\beta(2, 1) = \psi(2, 1) = 14$ , then by Theorem 3.3 and Proposition 2.3 we can get the number of spanning trees (spanning connected subgraphs, spanning forests, acyclic orientations) of the cylinder silicate graph  $CS_n$ .

**Corollary 3.4** For  $n \geq 2$ , (i) the number of spanning trees of  $CS_n$  is  $N_{ST}(CS_n) = 8n \cdot 16^{n-1}$ ; (ii) the number of spanning connected subgraphs of  $CS_n$  is  $N_{SCS}(CS_n) = (10n + 38) \cdot 38^{n-1}$ ; (iii) the number of acyclic orientations of  $CS_n$  is  $N_{AO}(CS_n) = 12^n(2^n - 2)$ ; (iv) the number of spanning forests of  $CS_n$  is  $N_{SF}(CS_n) = 38^n - 24^n$ .

In addition, it is easy to see that  $|V(CS_n)| = 3n$  and  $|E(CS_n)| = 6n$ . Then by (5) we have

$$\begin{aligned} \kappa(CS_n) &= \lim_{|V(CS_n)| \rightarrow \infty} \frac{\ln(N_{ST}(CS_n))}{|V(CS_n)|} = \lim_{n \rightarrow \infty} \frac{\ln(8n \cdot 16^{n-1})}{3n} \\ &= \lim_{n \rightarrow \infty} \frac{\ln(16^{n-1}) + \ln(8n)}{3n} \\ &= \lim_{n \rightarrow \infty} \frac{(n-1) \ln 16}{3n} \\ &= \frac{2 \ln 4}{3} \approx 0.924196. \end{aligned} \tag{7}$$

**Remark** The Eqs. (6) and (7) imply that the linear silicate chain  $LS_n$  and cyclic silicate molecular graph  $CS_n$  have the same spanning tree entropy. Similar phenomena also occur in the matching entropy of  $LS_n$  and  $CS_n$  [34].

### 3.3 The Tutte polynomial of double silicate molecular chain $DS_n$

Now, we consider the Tutte polynomial of double silicate molecular chain  $DS_n$ . The configurations of double silicate molecular chains  $DS_n$  for small  $n$  are shown in Figs. 3 and 4. In order to get the Tutte polynomial of  $DS_n$ , we need some auxiliary graphs. Let  $AS_n$  be the graph which is obtained from  $DS_n$  by identifying the two rightmost vertices, that is  $AS_n = DS_n / \{u, v\}$ , where  $u$  and  $v$  are the two rightmost vertices of  $DS_n$ . The graph  $AS_5$  and other two auxiliary graphs  $F$  and  $Q$  are illustrated in Fig. 5.

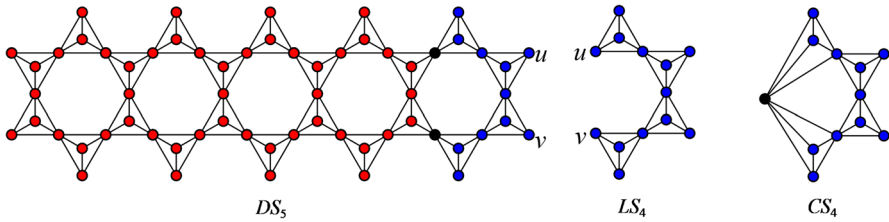


Fig. 4 Showing that  $DS_5 = DS_4 : LS_4$ , and the graphs  $LS_4$  and  $CS_4$

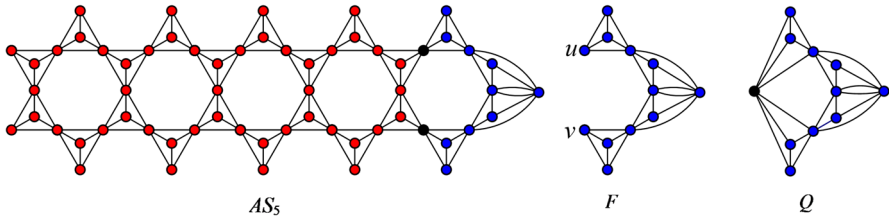


Fig. 5 Showing that  $AS_5 = DS_4 : F$ , and the graphs  $F$  and  $Q$

**Lemma 3.5** For  $n \geq 1$ , we have

$$T(DS_n; x, y) = f_1(x, y) \cdot T(AS_{n-1}; x, y) + f_2(x, y) \cdot T(DS_{n-1}; x, y), \quad (8)$$

where  $f_1(x, y) = (2+x^2+4y+3y^2+y^3+x(3+2y))^4$  and  $f_2(x, y) = 13x^{10} + x^{11} + x^9(75+16y) + x^8(255+168y+12y^2+4y^3) + x^7(575+768y+216y^2+40y^3) + 8(1+y)^6(2+4y+6y^2+4y^3+y^4) + x^6(923+2032y+1284y^2+316y^3+48y^4) + 4x(1+y)^3(28+108y+204y^2+224y^3+132y^4+36y^5+3y^6) + x^5(1109+3504y+3852y^2+1756y^3+414y^4+36y^5+6y^6) + x^4(1025+4200y+6840y^2+5336y^3+2058y^4+444y^5+42y^6) + 2x^2(1+y)^2(180+696y+1248y^2+1196y^3+563y^4+120y^5+14y^6+2y^7) + x^3(720+3584y+7740y^2+9004y^3+5802y^4+2028y^5+402y^6+48y^7)$ .

**Proof** The same as before, we use  $G : H$  to denote the graph obtained from  $G$  and  $H$  such that they have only two common vertices. By analyzing the structural characteristics of the double silicate molecular graph, we can find that  $DS_n$  can be constructed by the way of that  $DS_n = DS_{n-1} : LS_4$  and assume that  $V(DS_{n-1}) \cap V(LS_4) = \{u, v\}$ . Then one can see that  $LS_4/\{u, v\} = CS_4$  and  $DS_{n-1}/\{u, v\} = AS_{n-1}$ . Thus, from Proposition 2.2 and some simplifications, the desired result can be obtained.  $\square$

**Lemma 3.6** For  $n \geq 1$ , we have

$$T(AS_n; x, y) = g_1(x, y) \cdot T(AS_{n-1}; x, y) + g_2(x, y) \cdot T(DS_{n-1}; x, y), \quad (9)$$

where  $g_1(x, y) = (2+x^2+4y+3y^2+y^3+x(3+2y))^2(8+2x^3+24y+33y^2+31y^3+23y^4+13y^5+5y^6+y^7) + x^2(10+8y+3y^2+y^3) + 2x(8+14y+12y^2+8y^3+4y^4+y^5)$



and  $g_2(x, y) = x^{10} + x^9(13 + y) + x^8(75 + 25y + 4y^2) + x^7(255 + 199y + 58y^2 + 12y^3 + 2y^4) + x^6(574 + 811y + 412y^2 + 150y^3 + 30y^4 + 4y^5) + x^5(912 + 2004y + 1663y^2 + 851y^3 + 293y^4 + 63y^5 + 5y^6 + y^7) + x^4(1058 + 3252y + 4047y^2 + 2899y^3 + 1464y^4 + 477y^5 + 100y^6 + 11y^7) + (1 + y)^3(32 + 128y + 260y^2 + 336y^3 + 308y^4 + 216y^5 + 113y^6 + 38y^7 + 6y^8) + x(1 + y)^2(192 + 752y + 1424y^2 + 1664y^3 + 1362y^4 + 840y^5 + 363y^6 + 89y^7 + 8y^8) + x^3(896 + 3572y + 6139y^2 + 6109y^3 + 4138y^4 + 2028y^5 + 650y^6 + 128y^7 + 16y^8) + x^2(528 + 2600y + 5777y^2 + 7663y^3 + 6885y^4 + 4528y^5 + 2183y^6 + 700y^7 + 132y^8 + 16y^9 + 2y^{10})$ .

**Proof** One can see that the graph  $AS_n$  can be constructed by the way of that  $AS_n = DS_{n-1} : F$  and assume that  $V(DS_{n-1}) \cap V(F) = \{u, v\}$ . Then we can find that  $DS_{n-1}/\{u, v\} = AS_{n-1}$ ,  $F/\{u, v\} = Q$ ,  $LS_4/\{u, v\} = CS_4$  and  $DS_{n-1}/\{u, v\} = AS_{n-1}$ . For the Tutte polynomials of the small graphs  $F$  and  $Q$ , one can get  $T(F; x, y) = (3x^2 + x^3 + x(2 + 4y) + y(2 + 3y + y^2))^2(x^5 + x^4(6 + y) + x^3(13 + 10y + 4y^2) + y(1 + y)^2(4 + 4y + 4y^2 + 3y^3 + y^4) + x^2(12 + 25y + 16y^2 + 10y^3 + 2y^4) + 2x(2 + 10y + 14y^2 + 11y^3 + 7y^4 + 2y^5))$  and  $T(Q; x, y) = x^{10} + x^9(13 + y) + x^8(75 + 25y + 4y^2) + x^7(253 + 201y + 58y^2 + 12y^3 + 2y^4) + x^6(552 + 817y + 425y^2 + 152y^3 + 31y^4 + 4y^5) + x^5(810 + 1950y + 1725y^2 + 907y^3 + 319y^4 + 73y^5 + 7y^6 + y^7) + x^4(800 + 2886y + 4015y^2 + 3123y^3 + 1687y^4 + 613y^5 + 158y^6 + 25y^7 + y^8) + x^3(512 + 2648y + 5433y^2 + 6189y^3 + 4738y^4 + 2666y^5 + 1080y^6 + 328y^7 + 74y^8 + 8y^9) + y(1 + y)^3(32 + 128y + 244y^2 + 304y^3 + 288y^4 + 216y^5 + 129y^6 + 63y^7 + 25y^8 + 7y^9 + y^{10}) + x(1 + y)^2(32 + 320y + 932y^2 + 1440y^3 + 1500y^4 + 1194y^5 + 737y^6 + 355y^7 + 138y^8 + 40y^9 + 6y^{10}) + x^2(192 + 1424y + 4152y^2 + 6725y^3 + 7177y^4 + 5630y^5 + 3390y^6 + 1566y^7 + 567y^8 + 160y^9 + 29y^{10} + 2y^{11})$  by applying formula (1) directly. Thus, from Proposition 2.2 and some simplifications, the desired result can be obtained.  $\square$

**Lemma 3.7** For  $n \geq 1$ , we have

$$T(DS_{n+1}; x, y) = \Psi(x, y)T(DS_n; x, y) + \Phi(x, y)T(DS_{n-1}; x, y), \quad (10)$$

where  $\Psi(x, y) = 13x^{10} + x^{11} + x^9(75 + 16y) + x^8(255 + 168y + 12y^2 + 4y^3) + x^7(577 + 768y + 216y^2 + 40y^3) + x^6(945 + 2048y + 1287y^2 + 317y^3 + 48y^4) + x^5(1211 + 3660y + 3946y^2 + 1794y^3 + 426y^4 + 38y^5 + 6y^6) + x^4(1283 + 4824y + 7496y^2 + 5768y^3 + 2267y^4 + 517y^5 + 57y^6 + y^7) + 2x^3(552 + 2446y + 4877y^2 + 5469y^3 + 3568y^4 + 1362y^5 + 334y^6 + 57y^7 + 4y^8) + 2x(1 + y)^2(136 + 568y + 1166y^2 + 1510y^3 + 1297y^4 + 744y^5 + 299y^6 + 94y^7 + 23y^8 + 3y^9) + (1 + y)^3(48 + 208y + 452y^2 + 640y^3 + 636y^4 + 452y^5 + 237y^6 + 98y^7 + 33y^8 + 8y^9 + y^{10}) + x^2(696 + 3624y + 8777y^2 + 12851y^3 + 12189y^4 + 7565y^5 + 3108y^6 + 908y^7 + 209y^8 + 33y^9 + 2y^{10})$  and  $\Phi(x, y) = -(x^5 + 2x^4(3 + y) + x^3(13 + 14y + 3y^2 + y^3) + y(1 + y)^2(4 + 6y + 4y^2 + y^3) + 2x^2(6 + 15y + 10y^2 + 2y^3) + x(4 + 22y + 35y^2 + 23y^3 + 6y^4))^2(x^8 + x^7(11 + 3y + 3y^2 + y^3) + x^6(51 + 35y + 27y^2 + 21y^3 + 8y^4 + 2y^5) + x^5(129 + 165y + 125y^2 + 123y^3 + 79y^4 + 27y^5 + 5y^6 + y^7) + y(1 + y)^3(16 + 32y + 32y^2 + 32y^3 + 32y^4 + 23y^5 + 10y^6 + 2y^7) + x^4(192 + 405y + 377y^2 + 363y^3 + 326y^4 + 177y^5 + 52y^6 + 7y^7) + x(1 + y)^2(16 + 112y + 176y^2 + 168y^3 + 172y^4 + 156y^5 + 93y^6 + 31y^7 + 4y^8) +$

$$2x^3(84 + 276y + 358y^2 + 344y^3 + 345y^4 + 273y^5 + 137y^6 + 41y^7 + 6y^8) + x^2(80 + 408y + 776y^2 + 876y^3 + 871y^4 + 820y^5 + 585y^6 + 278y^7 + 84y^8 + 16y^9 + 2y^{10}).$$

**Proof** From (8), we have

$$T(AS_{n-1}; x, y) = \frac{1}{f_1(x, y)} T(DS_n) - \frac{f_2(x, y)}{f_1(x, y)} T(DS_{n-1}; x, y) \quad (11)$$

and

$$T(AS_n; x, y) = \frac{1}{f_1(x, y)} T(DS_{n+1}) - \frac{f_2(x, y)}{f_1(x, y)} T(DS_n; x, y). \quad (12)$$

If we plug (11) and (12) back into (9), then

$$\begin{aligned} T(DS_{n+1}; x, y) &= (g_1(x, y) + f_2(x, y))T(DS_n; x, y) \\ &\quad + (f_1(x, y)g_2(x, y) - g_1(x, y)f_2(x, y))T(DS_{n-1}; x, y) \\ &= \Psi(x, y)T(DS_n; x, y) + \Phi(x, y)T(DS_{n-1}; x, y), \end{aligned}$$

where  $\Psi(x, y) = g_1(x, y) + f_2(x, y)$  and  $\Phi(x, y) = f_1(x, y)g_2(x, y) - g_1(x, y)f_2(x, y)$ . Hence, the desired result follows.  $\square$

Noting that the initial conditions  $T(DS_0; x, y) = T(K_4 \cdot K_4; x, y) = (3x^2 + x^3 + x(2 + 4y) + y(2 + 3y + y^2))^2$ ,  $T(DS_1; x, y) = T(CS_6; x, y) = (2 + x^2 + 4y + 3y^2 + y^3 + x(3 + 2y))^4(x^5 + x^4(6 + y) + x^3(13 + 10y + 4y^2) + y(1 + y)^2(4 + 4y + 4y^2 + 3y^3 + y^4) + x^2(12 + 25y + 16y^2 + 10y^3 + 2y^4) + 2x(2 + 10y + 14y^2 + 11y^3 + 7y^4 + 2y^5)) + (3x^2 + x^3 + x(2 + 4y) + y(2 + 3y + y^2))^2(13x^{10} + x^{11} + x^9(75 + 16y) + x^8(255 + 168y + 12y^2 + 4y^3) + x^7(575 + 768y + 216y^2 + 40y^3) + 8(1 + y)^6(2 + 4y + 6y^2 + 4y^3 + y^4) + x^6(923 + 2032y + 1284y^2 + 316y^3 + 48y^4) + 4x(1 + y)^3(28 + 108y + 204y^2 + 224y^3 + 132y^4 + 36y^5 + 3y^6) + x^5(1109 + 3504y + 3852y^2 + 1756y^3 + 414y^4 + 36y^5 + 6y^6) + x^4(1025 + 4200y + 6840y^2 + 5336y^3 + 2058y^4 + 444y^5 + 42y^6) + 2x^2(1 + y)^2(180 + 696y + 1248y^2 + 1196y^3 + 563y^4 + 120y^5 + 14y^6 + 2y^7) + x^3(720 + 3584y + 7740y^2 + 9004y^3 + 5802y^4 + 2028y^5 + 402y^6 + 48y^7))$  and combining the characteristic equation of (10), one can derive the closed-form expression of the Tutte polynomial of  $DS_n$ .

**Theorem 3.8** *The Tutte polynomial of  $DS_n$  is given by*

$$T(DS_n; x, y) = \frac{2\lambda - \mu(\Psi - \sqrt{\Delta})}{\Delta + \Psi\sqrt{\Delta}} \left( \frac{\Psi + \sqrt{\Delta}}{2} \right)^{n+1} + \frac{2\lambda - \mu(\Psi + \sqrt{\Delta})}{\Delta - \Psi\sqrt{\Delta}} \left( \frac{\Psi - \sqrt{\Delta}}{2} \right)^{n+1},$$

where  $\mu = \mu(x, y) = T(DS_0; x, y)$ ,  $\lambda = \lambda(x, y) = T(DS_1; x, y)$ ,  $\Psi = \Psi(x, y)$  and  $\Delta = \Delta(x, y) = \Psi(x, y)^2 + 4\Phi(x, y)$ .

If we take  $x \in \{1, 2\}$  and  $y \in \{0, 1, 2\}$ , then it is easy to obtain that

- $\Psi(1, 1) = 196608$ ,  $\Phi(1, 1) = -1073741824$ ,  $\mu(1, 1) = 256$ ,  $\lambda(1, 1) = 50331648$  and  $\Delta(1, 1) = 34359738368$ .

- $\Psi(1, 2) = 5377456$ ,  $\Phi(1, 2) = -1210396426368$ ,  $\mu(1, 2) = 1444$ ,  $\lambda(1, 2) = 7765046464$  and  $\Delta(1, 2) = 24075447326464$ .
- $\Psi(2, 0) = 324864$ ,  $\Phi(2, 0) = -1146617856$ ,  $\mu(2, 0) = 576$ ,  $\lambda(2, 0) = 185131008$  and  $\Delta(2, 0) = 100950147072$ .
- $\Psi(2, 1) = 2001040$ ,  $\Phi(2, 1) = -100601100288$ ,  $\mu(2, 1) = 1444$ ,  $\lambda(2, 1) = 2819833408$  and  $\Delta(2, 1) = 3601756680448$ .

Thus, from Proposition 2.3 and Theorem 3.8 we have

**Corollary 3.9**

(i) *The number of spanning trees of  $DS_n$  is*

$$N_{ST}(DS_n) = \frac{(98304+65536\sqrt{2})^{n+1}}{512\sqrt{2}} - \frac{(98304-65536\sqrt{2})^{n+1}}{512\sqrt{2}}.$$

(ii) *The number of spanning connected subgraphs of  $DS_n$  is*

$$N_{SCS}(DS_n) = \frac{(54872(\sqrt{1999}+49))^{n+1}}{76\sqrt{1999}} - \frac{(54872(\sqrt{1999}-49))^{n+1}}{76\sqrt{1999}}.$$

(iii) *The number of acyclic orientations of  $DS_n$  is*

$$N_{AO}(DS_n) = \frac{15552(\sqrt{2113}+46)(3456(\sqrt{2113}+47))^{n+1}}{8771328\sqrt{2113}+94044716119} - \frac{15552(\sqrt{2113}-46)(3456(\sqrt{2113}-47))^{n+1}}{8771328\sqrt{2113}-94044716119}.$$

(iv) *The number of spanning forests of  $DS_n$  is*

$$N_{SF}(DS_n) = \frac{(361\sqrt{14069362033}+42971329)(8(\sqrt{14069362033}+125065))^{n+1}}{500260\sqrt{14069362033}+376178864476} - \frac{(361\sqrt{14069362033}-42971329)(8(\sqrt{14069362033}-125065))^{n+1}}{500260\sqrt{14069362033}-376178864476}.$$

It is easy to check that the number of vertices and the number of edges of  $DS_n$  are  $|V(DS_n)| = 11n + 7$  and  $|E(DS_n)| = 24n + 12$ , respectively. Then by (5) we have

$$\begin{aligned} \kappa(DS_n) &= \lim_{|V(DS_n)| \rightarrow \infty} \frac{\ln(N_{ST}(DS_n))}{|V(DS_n)|} \\ &= \lim_{n \rightarrow \infty} \frac{\ln\left(\frac{(98304+65536\sqrt{2})^{n+1}}{512\sqrt{2}} - \frac{(98304-65536\sqrt{2})^{n+1}}{512\sqrt{2}}\right)}{11n + 7} \\ &= \lim_{n \rightarrow \infty} \frac{\ln\left(\frac{(98304+65536\sqrt{2})^{n+1}}{512\sqrt{2}}\right) + \ln\left(1 - \left(\frac{98304-65536\sqrt{2}}{98304+65536\sqrt{2}}\right)^{n+1}\right)}{11n + 7} \end{aligned}$$

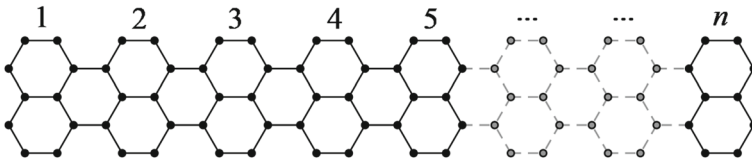


Fig. 6 The benzenoid system  $R_n$

$$\begin{aligned}
 &= \lim_{n \rightarrow \infty} \frac{(n+1) \ln(98304 + 65536\sqrt{2})}{11n + 7} \\
 &= \frac{\ln(98304 + 65536\sqrt{2})}{11} \approx 1.10545.
 \end{aligned}$$

## 4 The Tutte polynomials of three classes of benzenoid systems

In this section, we consider the Tutte polynomials of three classes of pericondensed benzenoid systems which are respectively illustrated in Figs. 6, 8 and 10. Some previous computation results for these pericondensed benzenoid systems can be found in [8, 38, 41].

### 4.1 The Tutte polynomial of benzenoid system $R_n$

In this subsection, we devote to get the Tutte polynomial of benzenoid system  $R_n$ . Let  $AR_n$  be the graph obtained from  $R_n$  by identifying the two rightmost vertices. The graphs  $AR_1$ ,  $AR_2$  and  $AR_4$  are shown in Fig. 7.

**Lemma 4.1** *The Tutte polynomial of  $R_n$  can be expressed by*

$$T(R_n; x, y) = h_1(x, y)T(AR_{n-1}; x, y) + h_2(x, y)T(R_{n-1}; x, y), \quad (13)$$

where  $h_1(x, y) = 6x^8 + 3x^9 + x^{10} + 2x^6(6+y) + x^7(9+y) + 4x^4(3+2y) + x^5(13+5y) + y(2+3y+y^2) + 2x^2(3+4y+y^2) + x^3(9+9y+2y^2) + x(2+7y+3y^2)$  and  $h_2(x, y) = (1+x)(2+8x^5+6x^6+4x^7+2x^8+x^9+3y+y^2+2x(2+y)+2x^3(4+y)+2x^4(4+y)+x^2(6+4y))$ .

**Proof** We find that the benzenoid system  $R_n$  can be established by the way of that  $R_n = R_{n-1} : J$  and assume the two common vertices of the graphs  $R_{n-1}$  and  $J$  are  $u$  and  $v$ , where the graph  $J$  is shown in Figure 7. Then it is not difficult to see that  $J/\{u, v\} = K$  and  $R_{n-1}/\{u, v\} = AR_{n-1}$ , the graph  $K$  is also shown in Figure 7. Furthermore, one can get that  $T(J; x, y) = x^2(x+x^2+x^3+x^4+x^5+x^6+x^7+x^8+x^9+y+(x+x^2+x^3+x^4+y)^2)$  and  $T(K; x, y) = 6x^8+3x^9+x^{10}+2x^6(6+y)+x^7(9+y)+4x^4(3+2y)+x^5(13+5y)+y(2+3y+y^2)+2x^2(3+4y+y^2)+x^3(9+9y+2y^2)+x(2+7y+3y^2)$ . Thus, by the use of Proposition 2.2 we have

$$T(R_n; x, y) = \frac{(x-1)T(K; x, y) - T(J; x, y)}{xy - x - y} T(AR_{n-1}; x, y)$$

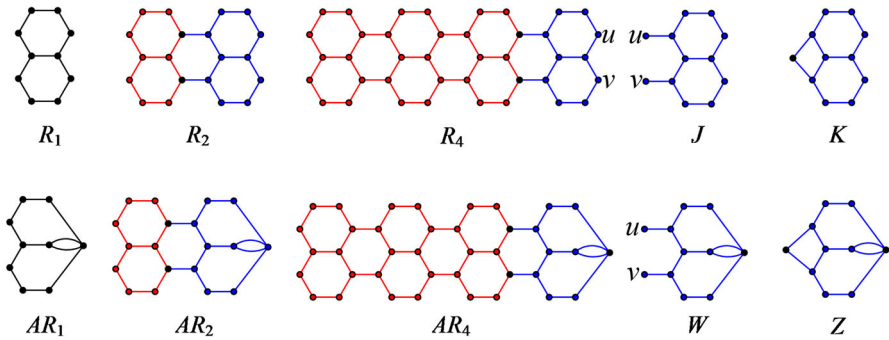


Fig. 7 Showing that  $R_n = R_{n-1} : J$  and  $AR_n = R_{n-1} : W$ , and the graphs  $J, K, W$  and  $Z$

$$\begin{aligned}
 &+ \frac{(y - 1)T(J; x, y) - T(K; x, y)}{xy - x - y} T(R_{n-1}; x, y) \\
 &= h_1(x, y)T(AR_{n-1}; x, y) + h_2(x, y)T(R_{n-1}; x, y),
 \end{aligned}$$

where  $h_1(x, y) = \frac{(x-1)T(K;x,y)-T(J;x,y)}{xy-x-y} = 6x^8 + 3x^9 + x^{10} + 2x^6(6 + y) + x^7(9 + y) + 4x^4(3 + 2y) + x^5(13 + 5y) + y(2 + 3y + y^2) + 2x^2(3 + 4y + y^2) + x^3(9 + 9y + 2y^2) + x(2 + 7y + 3y^2)$  and  $h_2(x, y) = \frac{(y-1)T(J;x,y)-T(K;x,y)}{xy-x-y} = (1 + x)(2 + 8x^5 + 6x^6 + 4x^7 + 2x^8 + x^9 + 3y + y^2 + 2x(2 + y) + 2x^3(4 + y) + 2x^4(4 + y) + x^2(6 + 4y))$ . □

**Lemma 4.2** *The Tutte polynomial of  $AR_n$  can be expressed by*

$$T(AR_n; x, y) = s_1(x, y)T(AR_{n-1}; x, y) + s_2(x, y)T(R_{n-1}; x, y), \tag{14}$$

where  $s_1(x, y) = x^6 + x^5(2 + y) + (1 + y)^2(2 + y) + x^4(3 + 2y) + x^3(4 + 3y) + 2x^2(3 + 3y + y^2) + x(5 + 7y + 2y^2)$  and  $s_2(x, y) = x^9 + 3x^7(2 + y) + (1 + y)^2(2 + y) + 4x^3(2 + y)^2 + x^8(3 + y) + 2x^6(5 + 3y) + 2x^5(7 + 5y) + 2x^4(8 + 7y + y^2) + x^2(13 + 17y + 6y^2) + x(7 + 12y + 6y^2 + y^3)$ .

**Proof** One can find that the graph  $AR_n$  can be constructed by the way of that  $AR_n = R_{n-1} : W$ , where the graph  $W$  is illustrated in Figure 7. If we set  $V(R_{n-1}) \cap V(W) = \{u, v\}$ , then it can be seen that  $R_{n-1}/\{u, v\} = AR_{n-1}$  and  $W/\{u, v\} = Z$ , the graph  $Z$  is also illustrated in Figure 7. By using the formula (1), it can be computed that  $T(W; x, y) = x^2((1 + y)(x + x^2 + x^3 + y)^2 + (1 + x + y)(x + x^2 + x^3 + x^4 + x^5 + x^6 + x^7 + y))$  and  $T(Z; x, y) = x^9 + 3x^7(2 + y) + y(1 + y)^2(2 + y) + x^8(3 + y) + x^6(9 + 7y) + x^5(12 + 11y + y^2) + x^4(13 + 15y + 4y^2) + x^3(12 + 17y + 7y^2) + x^2(7 + 17y + 10y^2 + 2y^3) + x(2 + 10y + 11y^2 + 3y^3)$ . Moreover, by Proposition 2.2 we have

$$\begin{aligned}
 T(AR_n; x, y) &= T(R_{n-1} : W; x, y) \\
 &= \frac{(x - 1)T(Z; x, y) - T(W; x, y)}{xy - x - y} T(AR_{n-1}; x, y)
 \end{aligned}$$

$$+ \frac{(y-1)T(W; x, y) - T(Z; x, y)}{xy - x - y} T(R_{n-1}; x, y) \\ = s_1(x, y)T(AR_{n-1}; x, y) + s_2(x, y)T(R_{n-1}; x, y),$$

where  $s_1(x, y) = \frac{(x-1)T(Z; x, y) - T(W; x, y)}{xy - x - y} = x^6 + x^5(2 + y) + (1 + y)^2(2 + y) + x^4(3 + 2y) + x^3(4 + 3y) + 2x^2(3 + 3y + y^2) + x(5 + 7y + 2y^2)$  and  $s_2(x, y) = \frac{(y-1)T(W; x, y) - T(Z; x, y)}{xy - x - y} = x^9 + 3x^7(2 + y) + (1 + y)^2(2 + y) + 4x^3(2 + y)^2 + x^8(3 + y) + 2x^6(5 + 3y) + 2x^5(7 + 5y) + 2x^4(8 + 7y + y^2) + x^2(13 + 17y + 6y^2) + x(7 + 12y + 6y^2 + y^3)$ .  $\square$

**Lemma 4.3** For  $n \geq 1$ , we have

$$T(R_{n+1}; x, y) = \Psi_1(x, y)T(R_n; x, y) + \Phi_1(x, y)T(R_{n-1}; x, y), \quad (15)$$

where  $\Psi_1(x, y) = 15x^6 + 10x^7 + 6x^8 + 3x^9 + x^{10} + 9x^3(2 + y) + (1 + y)(2 + y)^2 + 3x^5(6 + y) + x^4(19 + 6y) + 2x^2(8 + 6y + y^2) + x(11 + 12y + 3y^2)$  and  $\Phi_1(x, y) = -(1 + x)(2 + 8x^5 + 6x^6 + 4x^7 + 2x^8 + x^9 + 3y + y^2 + 2x(2 + y) + 2x^3(4 + y) + 2x^4(4 + y) + x^2(6 + 4y))(x^6 + x^5(2 + y) + (1 + y)^2(2 + y) + x^4(3 + 2y) + x^3(4 + 3y) + 2x^2(3 + 3y + y^2) + x(5 + 7y + 2y^2)) + (6x^8 + 3x^9 + x^{10} + 2x^6(6 + y) + x^7(9 + y) + 4x^4(3 + 2y) + x^5(13 + 5y) + y(2 + 3y + y^2) + 2x^2(3 + 4y + y^2) + x^3(9 + 9y + 2y^2) + x(2 + 7y + 3y^2))(x^9 + 3x^7(2 + y) + (1 + y)^2(2 + y) + 4x^3(2 + y)^2 + x^8(3 + y) + 2x^6(5 + 3y) + 2x^5(7 + 5y) + 2x^4(8 + 7y + y^2) + x^2(13 + 17y + 6y^2) + x(7 + 12y + 6y^2 + y^3))$ .

**Proof** From (13), we have

$$T(AR_{n-1}; x, y) = \frac{1}{h_1(x, y)} T(R_n) - \frac{h_2(x, y)}{h_1(x, y)} T(R_{n-1}; x, y) \quad (16)$$

and

$$T(AR_n; x, y) = \frac{1}{h_1(x, y)} T(R_{n+1}) - \frac{h_2(x, y)}{h_1(x, y)} T(R_n; x, y). \quad (17)$$

If we plug (16) and (17) back into (14), we obtain

$$T(R_{n+1}; x, y) = (s_1(x, y) + h_2(x, y))T(R_n; x, y) + (h_1(x, y)s_2(x, y) - s_1(x, y)h_2(x, y))T(R_{n-1}; x, y) \\ = \Psi_1(x, y)T(R_n; x, y) + \Phi_1(x, y)T(R_{n-1}; x, y),$$

where  $\Psi_1(x, y) = s_1(x, y) + h_2(x, y)$  and  $\Phi_1(x, y) = h_1(x, y)s_2(x, y) - s_1(x, y)h_2(x, y)$ . Hence, the desired result follows.  $\square$

It is straightforward to get the initial conditions that  $T(R_1; x, y) = x + x^2 + x^3 + x^4 + x^5 + x^6 + x^7 + x^8 + x^9 + y + (x + x^2 + x^3 + x^4 + y)^2$  and  $T(R_2; x, y) = (1 + x)(x + x^2 + x^3 + x^4 + x^5 + x^6 + x^7 + x^8 + x^9 + y + (x + x^2 + x^3 + x^4 + y)^2)(2 + 8x^5 + 6x^6 + 4x^7 + 2x^8 + x^9 + 3y + y^2 + 2x(2 + y) + 2x^3(4 + y) + 2x^4(4 + y) +$

$x^2(6 + 4y) + ((1 + y)(x + x^2 + x^3 + y)^2 + (1 + x + y)(x + x^2 + x^3 + x^4 + x^5 + x^6 + x^7 + y))(6x^8 + 3x^9 + x^{10} + 2x^6(6 + y) + x^7(9 + y) + 4x^4(3 + 2y) + x^5(13 + 5y) + y(2 + 3y + y^2) + 2x^2(3 + 4y + y^2) + x^3(9 + 9y + 2y^2) + x(2 + 7y + 3y^2))$ , then together with the characteristic equation of (15) we obtain the exact expression of the Tutte polynomial of benzenoid system  $R_n$ .

**Theorem 4.4** *The Tutte polynomial of  $R_n$  is given by*

$$T(R_n; x, y) = \frac{2\lambda_1 - \mu_1(\Psi_1 - \sqrt{\Delta_1})}{\Delta_1 + \Psi_1\sqrt{\Delta_1}} \left( \frac{\Psi_1 + \sqrt{\Delta_1}}{2} \right)^n + \frac{2\lambda_1 - \mu_1(\Psi_1 + \sqrt{\Delta_1})}{\Delta_1 - \Psi_1\sqrt{\Delta_1}} \left( \frac{\Psi_1 - \sqrt{\Delta_1}}{2} \right)^n,$$

where  $\mu_1 = \mu_1(x, y) = T(R_1; x, y)$ ,  $\lambda_1 = \lambda_1(x, y) = T(R_2; x, y)$ ,  $\Psi_1 = \Psi_1(x, y)$  and  $\Delta_1 = \Delta_1(x, y) = \Psi_1(x, y)^2 + 4\Phi_1(x, y)$ .

Moreover, it can easily be calculated that

- $\Psi_1(1, 1) = 182$ ,  $\Phi_1(1, 1) = 17640$ ,  $\mu_1(1, 1) = 35$ ,  $\lambda_1(1, 1) = 11466$  and  $\Delta_1(1, 1) = 103684$ .
- $\Psi_1(1, 2) = 269$ ,  $\Phi_1(1, 2) = 56262$ ,  $\mu_1(1, 2) = 47$ ,  $\lambda_1(1, 2) = 30181$  and  $\Delta_1(1, 2) = 297409$ .
- $\Psi_1(2, 0) = 7450$ ,  $\Phi_1(2, 0) = 22367448$ ,  $\mu_1(2, 0) = 1922$ ,  $\lambda_1(2, 0) = 20291524$  and  $\Delta_1(2, 0) = 144972292$ .
- $\Psi_1(2, 1) = 7814$ ,  $\Phi_1(2, 1) = 37822512$ ,  $\mu_1(2, 1) = 1984$ ,  $\lambda_1(2, 1) = 25635588$  and  $\Delta_1(2, 1) = 212348644$ .

Then by Theorem 4.4 and Proposition 2.3 we can get the number of spanning trees (spanning connected subgraphs, spanning forests, acyclic orientations) of the benzenoid system  $R_n$ .

**Corollary 4.5**

- (i) *The number of spanning trees of  $R_n$  is  $N_{ST}(R_n) = \frac{71 \times 252^n}{414} + \frac{27 \times (-70)^n}{230}$ .*
- (ii) *The number of spanning connected subgraphs of  $R_n$  is*

$$N_{SCS}(R_n) = \left( \frac{2923}{18754} + \frac{13593}{18754} \sqrt{\frac{7}{42487}} \right) \left( \frac{269 + \sqrt{297409}}{2} \right)^n + \left( \frac{2923}{18754} - \frac{13593}{18754} \sqrt{\frac{7}{42487}} \right) \left( \frac{269 - \sqrt{297409}}{2} \right)^n.$$

- (iii) *The number of acyclic orientations of  $R_n$  is*

$$N_{AO}(R_n) = \frac{(373289\sqrt{36243073} + 1296388166)(3725 + \sqrt{36243073})^n}{2795931\sqrt{36243073}} + \frac{(373289\sqrt{36243073} - 1296388166)(3725 - \sqrt{36243073})^n}{2795931\sqrt{36243073}}.$$

- (iv) *The number of spanning forests of  $R_n$  is*

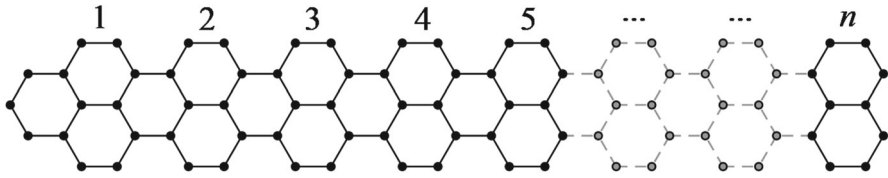


Fig. 8 The benzenoid system  $M_n$

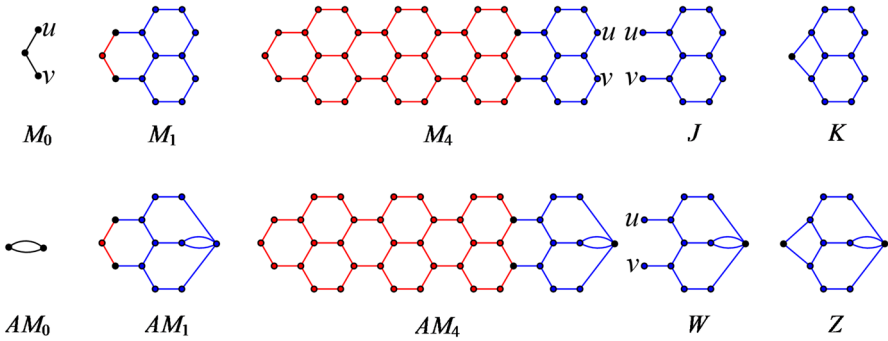


Fig. 9 Showing that  $M_n = M_{n-1} : J$  and  $AM_n = M_{n-1} : W$ , and the graphs  $M_0, AM_0, J, K, W$  and  $Z$

$$N_{SF}(R_n) = \frac{(51697\sqrt{53087161} + 180876269)(3907 + \sqrt{53087161})^n}{385944\sqrt{53087161}} + \frac{(51697\sqrt{53087161} - 180876269)(3907 - \sqrt{53087161})^n}{385944\sqrt{53087161}}$$

It is easy to check that the number of vertices and the number of edges of  $R_n$  are  $|V(R_n)| = 10n$  and  $|E(R_n)| = 13n - 2$ , respectively. Then by (5)

$$\begin{aligned} \kappa(R_n) &= \lim_{|V(R_n)| \rightarrow \infty} \frac{\ln(N_{ST}(R_n))}{|V(R_n)|} = \lim_{n \rightarrow \infty} \frac{\ln\left(\frac{71 \times 252^n}{414} + \frac{27 \times (-70)^n}{230}\right)}{10n} \\ &= \lim_{n \rightarrow \infty} \frac{\ln\left(\frac{71 \times 252^{n+1}}{414}\right) + \ln\left(1 + \frac{243}{355}\left(\frac{-70}{252}\right)^{n+1}\right)}{10n} \\ &= \lim_{n \rightarrow \infty} \frac{(n+1) \ln 252}{10n} = \frac{\ln 252}{10} \end{aligned}$$

### 4.2 The Tutte polynomial of benzenoid system $M_n$

Now, we consider the Tutte polynomial of benzenoid system  $M_n$ . The configuration of  $M_n$  is shown in Fig. 8. We let  $M_0 = P_3$ , the path with 3 vertices (see Fig. 9), for convenience. The graph  $AM_n$  is obtained from  $M_n$  by identifying the rightmost two vertices.



**Lemma 4.6** *The Tutte polynomial of  $M_n$  can be expressed by*

$$T(M_n; x, y) = h_1(x, y)T(AM_{n-1}; x, y) + h_2(x, y)T(M_{n-1}; x, y), \tag{18}$$

where  $h_1(x, y) = 6x^8 + 3x^9 + x^{10} + 2x^6(6 + y) + x^7(9 + y) + 4x^4(3 + 2y) + x^5(13 + 5y) + y(2 + 3y + y^2) + 2x^2(3 + 4y + y^2) + x^3(9 + 9y + 2y^2) + x(2 + 7y + 3y^2)$  and  $h_2(x, y) = (1 + x)(2 + 8x^5 + 6x^6 + 4x^7 + 2x^8 + x^9 + 3y + y^2 + 2x(2 + y) + 2x^3(4 + y) + 2x^4(4 + y) + x^2(6 + 4y))$ .

**Proof** It can be seen that  $M_n = M_{n-1} : J$  and assume that the common vertices of the graphs  $M_{n-1}$  and  $J$  is  $\{u, v\}$ . Then it is not difficult to get that  $J/\{u, v\} = K$  and  $M_{n-1}/\{u, v\} = AM_{n-1}$ , see Figure 9. Furthermore, one can get that  $T(J; x, y) = x^2(x + x^2 + x^3 + x^4 + x^5 + x^6 + x^7 + x^8 + x^9 + y + (x + x^2 + x^3 + x^4 + y)^2)$  and  $T(K; x, y) = 6x^8 + 3x^9 + x^{10} + 2x^6(6 + y) + x^7(9 + y) + 4x^4(3 + 2y) + x^5(13 + 5y) + y(2 + 3y + y^2) + 2x^2(3 + 4y + y^2) + x^3(9 + 9y + 2y^2) + x(2 + 7y + 3y^2)$ . Thus, by the use of Proposition 2.2 we have

$$\begin{aligned} T(M_n; x, y) &= \frac{(x - 1)T(K; x, y) - T(J; x, y)}{xy - x - y} T(AM_{n-1}; x, y) \\ &\quad + \frac{(y - 1)T(J; x, y) - T(K; x, y)}{xy - x - y} T(M_{n-1}; x, y) \\ &= h_1(x, y)T(AM_{n-1}; x, y) + h_2(x, y)T(M_{n-1}; x, y), \end{aligned}$$

where  $h_1(x, y) = \frac{(x-1)T(K;x,y)-T(J;x,y)}{xy-x-y} = 6x^8 + 3x^9 + x^{10} + 2x^6(6 + y) + x^7(9 + y) + 4x^4(3 + 2y) + x^5(13 + 5y) + y(2 + 3y + y^2) + 2x^2(3 + 4y + y^2) + x^3(9 + 9y + 2y^2) + x(2 + 7y + 3y^2)$  and  $h_2(x, y) = \frac{(y-1)T(J;x,y)-T(K;x,y)}{xy-x-y} = (1 + x)(2 + 8x^5 + 6x^6 + 4x^7 + 2x^8 + x^9 + 3y + y^2 + 2x(2 + y) + 2x^3(4 + y) + 2x^4(4 + y) + x^2(6 + 4y))$ . □

**Lemma 4.7** *The Tutte polynomial of  $AM_n$  can be expressed by*

$$T(AM_n; x, y) = s_1(x, y)T(AM_{n-1}; x, y) + s_2(x, y)T(M_{n-1}; x, y), \tag{19}$$

where  $s_1(x, y) = x^6 + x^5(2 + y) + (1 + y)^2(2 + y) + x^4(3 + 2y) + x^3(4 + 3y) + 2x^2(3 + 3y + y^2) + x(5 + 7y + 2y^2)$  and  $s_2(x, y) = x^9 + 3x^7(2 + y) + (1 + y)^2(2 + y) + 4x^3(2 + y)^2 + x^8(3 + y) + 2x^6(5 + 3y) + 2x^5(7 + 5y) + 2x^4(8 + 7y + y^2) + x^2(13 + 17y + 6y^2) + x(7 + 12y + 6y^2 + y^3)$ .

**Proof** One can find that the graph  $AM_n$  can be constructed by the way of that  $AM_n = M_{n-1} : W$ . If we set  $V(M_{n-1}) \cap V(W) = \{u, v\}$ , then it can be seen that  $M_{n-1}/\{u, v\} = AM_{n-1}$  and  $W/\{u, v\} = Z$ . By using the formula (1), it can be computed that  $T(W; x, y) = x^2((1 + y)(x + x^2 + x^3 + y)^2 + (1 + x + y)(x + x^2 + x^3 + x^4 + x^5 + x^6 + x^7 + y))$  and  $T(Z; x, y) = x^9 + 3x^7(2 + y) + y(1 + y)^2(2 + y) + x^8(3 + y) + x^6(9 + 7y) + x^5(12 + 11y + y^2) + x^4(13 + 15y + 4y^2) + x^3(12 +$

$17y + 7y^2) + x^2(7 + 17y + 10y^2 + 2y^3) + x(2 + 10y + 11y^2 + 3y^3)$ . Moreover, by Proposition 2.2 we have

$$\begin{aligned} T(AM_n; x, y) &= T(M_{n-1} : W; x, y) = \frac{(x-1)T(Z; x, y) - T(W; x, y)}{xy - x - y} T(AM_{n-1}; x, y) \\ &\quad + \frac{(y-1)T(W; x, y) - T(Z; x, y)}{xy - x - y} T(M_{n-1}; x, y) \\ &= s_1(x, y)T(AM_{n-1}; x, y) + s_2(x, y)T(M_{n-1}; x, y), \end{aligned}$$

where  $s_1(x, y) = \frac{(x-1)T(Z;x,y)-T(W;x,y)}{xy-x-y} = x^6 + x^5(2 + y) + (1 + y)^2(2 + y) + x^4(3 + 2y) + x^3(4 + 3y) + 2x^2(3 + 3y + y^2) + x(5 + 7y + 2y^2)$  and  $s_2(x, y) = \frac{(y-1)T(W;x,y)-T(Z;x,y)}{xy-x-y} = x^9 + 3x^7(2 + y) + (1 + y)^2(2 + y) + 4x^3(2 + y)^2 + x^8(3 + y) + 2x^6(5 + 3y) + 2x^5(7 + 5y) + 2x^4(8 + 7y + y^2) + x^2(13 + 17y + 6y^2) + x(7 + 12y + 6y^2 + y^3)$ .  $\square$

**Lemma 4.8** *The Tutte polynomial of  $M_n$  can be expressed by*

$$T(M_{n+1}; x, y) = \Psi_1(x, y)T(M_n; x, y) + \Phi_1(x, y)T(M_{n-1}; x, y). \tag{20}$$

**Proof** An argument similar to Lemma 4.3, one can obtain the desired result (20) by applying (18) and (19).  $\square$

On account of the initial conditions  $T(M_0; x, y) = x^2$  and  $T(M_1; x, y) = 4x^{11} + x^{12} + x^{10}(9 + y) + x^9(16 + 3y) + x^8(23 + 7y) + y^2(2 + 3y + y^2) + x^7(28 + 13y + y^2) + 2xy(2 + 5y + 2y^2) + x^6(29 + 21y + 2y^2) + x^5(26 + 27y + 5y^2) + x^4(19 + 27y + 10y^2) + 2x^2(2 + 8y + 6y^2 + y^3) + 2x^3(6 + 11y + 6y^2 + y^3)$ , and by using the characteristic equation of (20) we can get the Tutte polynomial of  $M_n$ .

**Theorem 4.9** *The Tutte polynomial of  $M_n$  is given by*

$$T(M_n; x, y) = \frac{2\eta - x^2(\Psi_1 - \sqrt{\Delta_1})}{\Delta_1 + \Psi_1\sqrt{\Delta_1}} \left(\frac{\Psi_1 + \sqrt{\Delta_1}}{2}\right)^{n+1} + \frac{2\eta - x^2(\Psi_1 + \sqrt{\Delta_1})}{\Delta_1 - \Psi_1\sqrt{\Delta_1}} \left(\frac{\Psi_1 - \sqrt{\Delta_1}}{2}\right)^{n+1},$$

where  $\eta = \eta(x, y) = T(M_1; x, y)$ ,  $\Psi_1 = \Psi_1(x, y)$  and  $\Delta_1 = \Delta_1(x, y) = \Psi_1(x, y)^2 + 4\Phi_1(x, y)$ .

Since it is also easy to get  $\eta(1, 1) = 378$ ,  $\eta(1, 2) = 773$ ,  $\eta(2, 0) = 42272$  and  $\eta(2, 1) = 51954$ , then from Theorem 4.9 and Proposition 2.3 we can get the number of spanning trees (spanning connected subgraphs, spanning forests, acyclic orientations) of the benzenoid system  $M_n$ .

**Corollary 4.10**

- (i) *The number of spanning trees of  $M_n$  is  $N_{ST}(M_n) = \frac{8 \times 252^{n+1}}{1449} + \frac{9 \times (-70)^{n+1}}{1610}$ .*
- (ii) *The number of spanning connected subgraphs of  $M_n$  is*

$$N_{SCS}(M_n) = \left(\frac{42}{9377} - \frac{1921}{9377\sqrt{297409}}\right) \left(\frac{269+\sqrt{297409}}{2}\right)^{n+1} + \left(\frac{42}{9377} + \frac{1921}{9377\sqrt{297409}}\right) \left(\frac{269-\sqrt{297409}}{2}\right)^{n+1}.$$

(iii) The number of acyclic orientations of  $M_n$  is

$$N_{AO}(M_n) = \frac{(1559\sqrt{36243073}+5376449)(3725+\sqrt{36243073})^{n+1}}{5591862\sqrt{36243073}} + \frac{(1559\sqrt{36243073}-5376449)(3725-\sqrt{36243073})^{n+1}}{5591862\sqrt{36243073}}.$$

(iv) The number of spanning forests of  $M_n$  is

$$N_{SF}(M_n) = \frac{(10349\sqrt{53087161}+35211481)(3907+\sqrt{53087161})^{n+1}}{37822512\sqrt{53087161}} + \frac{(10349\sqrt{53087161}-35211481)(3907-\sqrt{53087161})^{n+1}}{37822512\sqrt{53087161}}.$$

It is easy to check that the number of vertices and the number of edges of  $M_n$  are  $|V(M_n)| = 10n + 3$  and  $|E(M_n)| = 13n + 2$ , respectively. Then by (5), we have

$$\begin{aligned} \kappa(M_n) &= \lim_{|V(M_n)| \rightarrow \infty} \frac{\ln(N_{ST}(M_n))}{|V(M_n)|} \\ &= \lim_{n \rightarrow \infty} \frac{\ln\left(\frac{8 \times 252^{n+1}}{1449} + \frac{9 \times (-70)^{n+1}}{1610}\right)}{10n + 3} \\ &= \lim_{n \rightarrow \infty} \frac{\ln\left(\frac{8 \times 252^{n+1}}{1449}\right) + \ln\left(1 + \frac{81}{80} \left(\frac{-70}{252}\right)^{n+1}\right)}{10n + 6} \\ &= \lim_{n \rightarrow \infty} \frac{(n + 1) \ln 252}{10n + 3} \\ &= \frac{\ln 252}{10}. \end{aligned}$$

By Lemma 4.7, we can easily get the following result.

**Lemma 4.11** For  $n \geq 1$ , we have

$$T(AM_{n+1}; x, y) = \Psi_1(x, y)T(AM_n; x, y) + \Phi_1(x, y)T(AM_{n-1}; x, y). \tag{21}$$

It can be straightforward to get the initial conditions  $T(AM_0; x, y) = x + y$  and  $T(AM_1; x, y) = x^{11} + 3x^9(2 + y) + y(1 + y)^2(2 + y) + x^{10}(3 + y) + 5x^7(3 + 2y) + 2x^8(5 + 3y) + 2x^6(9 + 8y + y^2) + x^5(19 + 20y + 5y^2) + x^4(17 + 23y + 8y^2) + x^3(13 + 22y + 11y^2 + y^3) + x(2 + 10y + 11y^2 + 3y^3) + x^2(7 + 18y + 12y^2 + 3y^3)$ , then combing the the characteristic equation of (21) we can get the Tutte polynomial of  $AM_n$ .

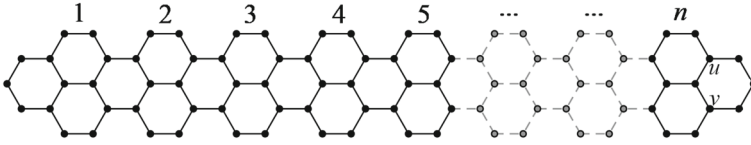


Fig. 10 The benzenoid system  $H_n$

**Theorem 4.12** *The Tutte polynomial of  $AM_n$  is given by*

$$T(AM_n; x, y) = \frac{2\omega - (x+y)(\Psi_1 - \sqrt{\Delta_1})}{\Delta_1 + \Psi_1 \sqrt{\Delta_1}} \left( \frac{\Psi_1 + \sqrt{\Delta_1}}{2} \right)^{n+1} + \frac{2\omega - (x+y)(\Psi_1 + \sqrt{\Delta_1})}{\Delta_1 - \Psi_1 \sqrt{\Delta_1}} \left( \frac{\Psi_1 - \sqrt{\Delta_1}}{2} \right)^{n+1},$$

where  $\omega = \omega(x, y) = T(AM_1; x, y)$ ,  $\Psi_1 = \Psi_1(x, y)$  and  $\Delta_1 = \Delta_1(x, y) = \Psi_1(x, y)^2 + 4\Phi_1(x, y)$ .

### 4.3 The Tutte polynomials of benzenoid system $H_n$

In this subsection, we derive the Tutte polynomials of benzenoid system  $H_n$  (see Fig. 10) by using the structural relation between  $H_n$  and  $M_n$ .

**Lemma 4.13** *The Tutte polynomials for  $H_n$ ,  $M_n$  and  $AM_n$  satisfy the following relation:*

$$T(H_n; x, y) = T(AM_n; x, y) + (1 + x + x^2 + x^3)T(M_n; x, y).$$

**Proof** From the structural feature of  $H_n$ , one can easily find that the benzenoid system  $H_n$  can be constructed by  $M_n$  and  $P_5$ , that is  $H_n = M_n : P_5$ . If we set  $V(M_n) \cap V(P_5) = \{u, v\}$ , then  $M_n / \{u, v\} = AM_n$  and  $P_5 / \{u, v\} = C_4$ . By using Proposition 2.2 we have

$$\begin{aligned} T(H_n; x, y) &= T(M_n : P_5; x, y) = \frac{(x-1)T(C_4; x, y) - T(P_5; x, y)}{xy - x - y} T(AM_n; x, y) \\ &\quad + \frac{(y-1)T(P_5; x, y) - T(C_4; x, y)}{xy - x - y} T(M_n; x, y) \\ &= \frac{(x-1)(y+x+x^2+x^3) - x^4}{xy - x - y} T(AM_n; x, y) \\ &\quad + \frac{(y-1)x^4 - (y+x+x^2+x^3)}{xy - x - y} T(M_n; x, y) \\ &= T(AM_n; x, y) + (1 + x + x^2 + x^3)T(M_n; x, y). \end{aligned}$$

Thus, we derive the desired result.  $\square$

According to Theorems 4.9, 4.12 and Lemma 4.13, the Tutte polynomial of benzenoid system  $H_n$  is straightforward.

**Theorem 4.14** *The Tutte polynomial of  $H_n$  is given by*

$$T(H_n; x, y) = \frac{2\theta - \vartheta(\Psi_1 - \sqrt{\Delta_1})}{\Delta_1 + \Psi_1 \sqrt{\Delta_1}} \left( \frac{\Psi_1 + \sqrt{\Delta_1}}{2} \right)^{n+1} + \frac{2\theta - \vartheta(\Psi_1 + \sqrt{\Delta_1})}{\Delta_1 - \Psi_1 \sqrt{\Delta_1}} \left( \frac{\Psi_1 - \sqrt{\Delta_1}}{2} \right)^{n+1},$$

where  $\vartheta = \vartheta(x, y) = x + x^2 + x^3 + x^4 + x^5 + y$  and  $\theta = \theta(x, y) = 5x^{14} + x^{15} + x^{13}(14 + y) + x^{12}(30 + 4y) + x^{11}(53 + 11y) + x^{10}(79 + 25y + y^2) + x^9(102 + 47y + 3y^2) + 2x^8(58 + 37y + 4y^2) + x^7(117 + 98y + 18y^2) + 4x^5(20 + 28y + 11y^2 + y^3) + y(2 + 7y + 7y^2 + 2y^3) + x^6(104 + 113y + 31y^2 + 2y^3) + x^4(52 + 92y + 52y^2 + 8y^3) + x(2 + 14y + 23y^2 + 10y^3 + y^4) + x^2(11 + 38y + 36y^2 + 12y^3 + y^4) + x^3(29 + 64y + 47y^2 + 12y^3 + y^4)$ .

One can obtain easily that  $\vartheta(1, 1) = 6, \vartheta(1, 2) = 7, \vartheta(2, 0) = 62, \vartheta(2, 1) = 63, \theta(1, 1) = 1820, \theta(1, 2) = 3785, \theta(2, 0) = 648920$  and  $\theta(2, 1) = 802438$ , then from Theorem 4.14 and Proposition 2.3 we can get the number of spanning trees (spanning connected subgraphs, spanning forests, acyclic orientations) of the benzenoid system  $H_n$ .

**Corollary 4.15**

- (i) *The number of spanning trees of  $H_n$  is  $N_{ST}(H_n) = \frac{40 \times 252^{n+1}}{1449} + \frac{11 \times (-70)^{n+1}}{805}$ .*
- (ii) *The number of spanning connected subgraphs of  $H_n$  is*

$$N_{SCS}(H_n) = \left( \frac{317}{18754} + \frac{46005}{18754\sqrt{297409}} \right) \left( \frac{269 + \sqrt{297409}}{2} \right)^{n+1} + \left( \frac{317}{18754} - \frac{46005}{18754\sqrt{297409}} \right) \left( \frac{269 - \sqrt{297409}}{2} \right)^{n+1}.$$

- (iii) *The number of acyclic orientations of  $H_n$  is*

$$N_{AO}(H_n) = \frac{(5195\sqrt{36243073} + 19170341)(3725 + \sqrt{36243073})^{n+1}}{1242636\sqrt{36243073}} + \frac{(5195\sqrt{36243073} - 19170341)(3725 - \sqrt{36243073})^{n+1}}{1242636\sqrt{36243073}}.$$

- (iv) *The number of spanning forests of  $H_n$  is*

$$N_{SF}(H_n) = \frac{(11077\sqrt{53087161} + 41822813)(3907 + \sqrt{53087161})^{n+1}}{2701608\sqrt{53087161}} + \frac{(11077\sqrt{53087161} - 41822813)(3907 - \sqrt{53087161})^{n+1}}{2701608\sqrt{53087161}}.$$

It is easy to check that the number of vertices and the number of edges of  $H_n$  are  $|V(H_n)| = 10n + 6$  and  $|E(H_n)| = 13n + 6$ , respectively. Then

$$\begin{aligned}
\kappa(H_n) &= \lim_{|V(H_n)| \rightarrow \infty} \frac{\ln(N_{ST}(H_n))}{|V(H_n)|} \\
&= \lim_{n \rightarrow \infty} \frac{\ln\left(\frac{40 \times 252^{n+1}}{1449} + \frac{11 \times (-70)^{n+1}}{805}\right)}{10n + 6} \\
&= \lim_{n \rightarrow \infty} \frac{\ln\left(\frac{40 \times 252^{n+1}}{1449}\right) + \ln\left(1 + \frac{99}{200} \left(\frac{-70}{252}\right)^{n+1}\right)}{10n + 6} \\
&= \lim_{n \rightarrow \infty} \frac{(n+1) \ln 252}{10n + 6} \\
&= \frac{\ln 252}{10}.
\end{aligned}$$

From above one can see that  $\kappa(R_n) = \kappa(M_n) = \kappa(H_n) = \frac{\ln 252}{10} \approx 0.552943$  which seems foreseeable due to their similar molecular structure.

## 5 Conclusion

In this paper, we have utilized combinatorial decomposition techniques to derive explicit closed-form analytic formulas for the Tutte polynomials of several important polycyclic chemical graphs, including three classes of typical silicate molecular graphs and three classes of pericondensed benzenoid systems. Our results have enabled us to determine the number of spanning trees, spanning connected subgraphs, spanning forests, and acyclic orientations for these graphs, as well as their corresponding spanning tree entropies. These findings provide valuable insights into the chemical and physical properties of silicates and benzenoid systems. We anticipate that the methodology employed in this paper can be applied to derive Tutte polynomials for almost all 2-connected polycyclic molecular graphs. However, our approach is not applicable to 3-connected networks, so it would be interesting to explore the Tutte polynomial for 3-connected chemical polycyclic networks in future research.

**Acknowledgements** The authors thank the anonymous referees for their valuable comments and suggestions. This work was supported by the National Natural Science Foundation of China (12201634), the Natural Science Foundation of Hunan Province (2023JJ30070) and the Education Department Foundation of Hunan Province (22B0828).

**Author contributions** The entire work from the design to its completion has been carried out by the author himself.

**Funding** This work was supported by the National Natural Science Foundation of China (Grant No. 12201634), the Education Department Foundation of Hunan Province (Grant No. 22B0828), the Natural Science Foundation of Hunan Province (Grant No. 2023JJ30070).

**Data availability** Data from this work can be available to other researchers in this field upon request to the author.

## Declarations

**Conflict of interest** The authors declare that they have no conflict of interest or other ethical conflicts concerning this paper.

**Ethical approval** Not applicable.

## Appendix

The Tutte polynomials for silicate molecular networks  $CS_3$ ,  $CS_4$ ,  $CS_5$ ,  $CS_6$ ,  $CS_7$  and  $CS_8$ .

$$T(CS_3; x, y) = (2 + 3x + x^2 + 2y)(2x + 3x^2 + x^3 + 2y + 4xy + 3y^2 + y^3)^2 + (2 + 3x + x^2 + 4y + 2xy + 3y^2 + y^3)(4x + 12x^2 + 13x^3 + 6x^4 + x^5 + 4y + 20xy + 25x^2y + 10x^3y + x^4y + 12y^2 + 28xy^2 + 16x^2y^2 + 4x^3y^2 + 16y^3 + 22xy^3 + 10x^2y^3 + 15y^4 + 14xy^4 + 2x^2y^4 + 11y^5 + 4xy^5 + 5y^6 + y^7);$$

$$T(CS_4; x, y) = (2x + 3x^2 + x^3 + 2y + 4xy + 3y^2 + y^3)^2(4 + 16x + 25x^2 + 19x^3 + 7x^4 + x^5 + 16y + 40xy + 32x^2y + 8x^3y + 24y^2 + 30xy^2 + 6x^2y^2 + 16y^3 + 6xy^3 + 2x^2y^3 + 4y^4) + (2 + 3x + x^2 + 4y + 2xy + 3y^2 + y^3)^2(4x + 12x^2 + 13x^3 + 6x^4 + x^5 + 4y + 20xy + 25x^2y + 10x^3y + x^4y + 12y^2 + 28xy^2 + 16x^2y^2 + 4x^3y^2 + 16y^3 + 22xy^3 + 10x^2y^3 + 15y^4 + 14xy^4 + 2x^2y^4 + 11y^5 + 4xy^5 + 5y^6 + y^7);$$

$$T(CS_5; x, y) = (2 + 3x + x^2 + 4y + 2xy + 3y^2 + y^3)^3(4x + 12x^2 + 13x^3 + 6x^4 + x^5 + 4y + 20xy + 25x^2y + 10x^3y + x^4y + 12y^2 + 28xy^2 + 16x^2y^2 + 4x^3y^2 + 16y^3 + 22xy^3 + 10x^2y^3 + 15y^4 + 14xy^4 + 2x^2y^4 + 11y^5 + 4xy^5 + 5y^6 + y^7) + (2x + 3x^2 + x^3 + 2y + 4xy + 3y^2 + y^3)^2(8 + 44x + 110x^2 + 165x^3 + 162x^4 + 105x^5 + 43x^6 + 10x^7 + x^8 + 48y + 216xy + 420x^2y + 450x^3y + 276x^4y + 90x^5y + 12x^6y + 132y^2 + 456xy^2 + 621x^2y^2 + 399x^3y^2 + 111x^4y^2 + 9x^5y^2 + 212y^3 + 512xy^3 + 419x^2y^3 + 129x^3y^3 + 21x^4y^3 + 3x^5y^3 + 210y^4 + 309xy^4 + 123x^2y^4 + 24x^3y^4 + 126y^5 + 90xy^5 + 18x^2y^5 + 42y^6 + 9xy^6 + 3x^2y^6 + 6y^7);$$

$$T(CS_6; x, y) = (2 + 3x + x^2 + 4y + 2xy + 3y^2 + y^3)^4(4x + 12x^2 + 13x^3 + 6x^4 + x^5 + 4y + 20xy + 25x^2y + 10x^3y + x^4y + 12y^2 + 28xy^2 + 16x^2y^2 + 4x^3y^2 + 16y^3 + 22xy^3 + 10x^2y^3 + 15y^4 + 14xy^4 + 2x^2y^4 + 11y^5 + 4xy^5 + 5y^6 + y^7) + (2x + 3x^2 + x^3 + 2y + 4xy + 3y^2 + y^3)^2(16 + 112x + 360x^2 + 720x^3 + 1025x^4 + 1109x^5 + 923x^6 + 575x^7 + 255x^8 + 75x^9 + 13x^{10} + x^{11} + 128y + 768xy + 2112x^2y + 3584x^3y + 4200x^4y + 3504x^5y + 2032x^6y + 768x^7y + 168x^8y + 16x^9y + 480y^2 + 2448xy^2 + 5640x^2y^2 + 7740x^3y^2 + 6840x^4y^2 + 3852x^5y^2 + 1284x^6y^2 + 216x^7y^2 + 12x^8y^2 + 1120y^3 + 4752xy^3 + 8776x^2y^3 + 9004x^3y^3 + 5336x^4y^3 + 1756x^5y^3 + 316x^6y^3 + 40x^7y^3 + 4x^8y^3 + 1800y^4 + 6096xy^4 + 8406x^2y^4 + 5802x^3y^4 + 2058x^4y^4 + 414x^5y^4 + 48x^6y^4 + 2064y^5 + 5232xy^5 + 4884x^2y^5 + 2028x^3y^5 + 444x^4y^5 + 36x^5y^5 + 1688y^6 + 2924xy^6 + 1634x^2y^6 + 402x^3y^6 + 42x^4y^6 + 6x^5y^6 + 960y^7 + 996xy^7 + 300x^2y^7 + 48x^3y^7 + 360y^8 + 180xy^8 + 36x^2y^8 + 80y^9 + 12xy^9 + 4x^2y^9 + 8y^{10});$$

$$T(CS_7; x, y) = (2 + 3x + x^2 + 4y + 2xy + 3y^2 + y^3)^5(4x + 12x^2 + 13x^3 + 6x^4 + x^5 + 4y + 20xy + 25x^2y + 10x^3y + x^4y + 12y^2 + 28xy^2 + 16x^2y^2 + 4x^3y^2 + 16y^3 + 22xy^3 + 10x^2y^3 + 15y^4 + 14xy^4 + 2x^2y^4 + 11y^5 + 4xy^5 + 5y^6 + y^7) + (2x + 3x^2 + x^3 + 2y + 4xy + 3y^2 + y^3)^2(32 + 272x + 1072x^2 + 2632x^3 + 4602x^4 + 6253x^5 + 6998x^6 + 6588x^7 + 5128x^8 + 3173x^9 + 1491x^{10} + 506x^{11} + 116x^{12} + 16x^{13} + x^{14} + 320y + 2400xy + 8320x^2y + 18000x^3y + 27860x^4y + 33390x^5y + 32030x^6y + 24330x^7y +$$

$$\begin{aligned}
& 14060x^8y + 5850x^9y + 1630x^{10}y + 270x^{11}y + 20x^{12}y + 1520y^2 + 10000xy^2 + \\
& 30360x^2y^2 + 57520x^3y^2 + 77375x^4y^2 + 78195x^5y^2 + 59485x^6y^2 + 32825x^7y^2 + \\
& 12345x^8y^2 + 2885x^9y^2 + 355x^{10}y^2 + 15x^{11}y^2 + 4560y^3 + 26160xy^3 + 69000x^2y^3 + \\
& 112400x^3y^3 + 126125x^4y^3 + 100185x^5y^3 + 55015x^6y^3 + 19835x^7y^3 + 4435x^8y^3 + \\
& 615x^9y^3 + 65x^{10}y^3 + 5x^{11}y^3 + 9680y^4 + 47960xy^4 + 107900x^2y^4 + 145570x^3y^4 + \\
& 127900x^4y^4 + 73450x^5y^4 + 26830x^6y^4 + 6180x^7y^4 + 930x^8y^4 + 80x^9y^4 + 15392y^5 + \\
& 64672xy^5 + 119952x^2y^5 + 126592x^3y^5 + 80672x^4y^5 + 31200x^5y^5 + 7500x^6y^5 + \\
& 1080x^7y^5 + 60x^8y^5 + 18840y^6 + 65080xy^6 + 94530x^2y^6 + 72620x^3y^6 + 31270x^4y^6 + \\
& 8000x^5y^6 + 1150x^6y^6 + 100x^7y^6 + 10x^8y^6 + 17880y^7 + 48480xy^7 + 51510x^2y^7 + \\
& 26670x^3y^7 + 7530x^4y^7 + 1170x^5y^7 + 120x^6y^7 + 13050y^8 + 26055xy^8 + 18615x^2y^8 + \\
& 6150x^3y^8 + 1110x^4y^8 + 90x^5y^8 + 7170y^9 + 9660xy^9 + 4230x^2y^9 + 910x^3y^9 + \\
& 70x^4y^9 + 10x^5y^9 + 2860y^{10} + 2290xy^{10} + 590x^2y^{10} + 80x^3y^{10} + 780y^{11} + 300xy^{11} + \\
& 60x^2y^{11} + 130y^{12} + 15xy^{12} + 5x^2y^{12} + 10y^{13});
\end{aligned}$$

$$\begin{aligned}
T(CS_8; x, y) = & (2 + 3x + x^2 + 4y + 2xy + 3y^2 + y^3)^6(4x + 12x^2 + 13x^3 + 6x^4 + \\
& x^5 + 4y + 20xy + 25x^2y + 10x^3y + x^4y + 12y^2 + 28x^2y^2 + 16x^3y^2 + 4x^4y^2 + 16y^3 + \\
& 22xy^3 + 10x^2y^3 + 15y^4 + 14xy^4 + 2x^2y^4 + 11y^5 + 4xy^5 + 5y^6 + y^7) + (2x + 3x^2 + \\
& x^3 + 2y + 4xy + 3y^2 + y^3)^2(64 + 640x + 2992x^2 + 8752x^3 + 18172x^4 + 29008x^5 + \\
& 37933x^6 + 42775x^7 + 42778x^8 + 37738x^9 + 28465x^{10} + 17647x^{11} + 8659x^{12} + \\
& 3241x^{13} + 886x^{14} + 166x^{15} + 19x^{16} + x^{17} + 768y + 6912xy + 28992x^2y + 76032x^3y + \\
& 142032x^4y + 205680x^5y + 245868x^6y + 251688x^7y + 220848x^8y + 161328x^9y + \\
& 94056x^{10}y + 41856x^{11}y + 13536x^{12}y + 2976x^{13}y + 396x^{14}y + 24x^{15}y + 4416y^2 + \\
& 35616xy^2 + 133536x^2y^2 + 313296x^3y^2 + 526116x^4y^2 + 688074x^5y^2 + 737064x^6y^2 + \\
& 654084x^7y^2 + 469464x^8y^2 + 260994x^9y^2 + 106818x^{10}y^2 + 30288x^{11}y^2 + 5448x^{12}y^2 + \\
& 528x^{13}y^2 + 18x^{14}y^2 + 16192y^3 + 116512xy^3 + 389152x^2y^3 + 814672x^3y^3 + \\
& 1222852x^4y^3 + 1417738x^5y^3 + 1305248x^6y^3 + 941468x^7y^3 + 511688x^8y^3 + \\
& 199538x^9y^3 + 53006x^{10}y^3 + 9176x^{11}y^3 + 1056x^{12}y^3 + 96x^{13}y^3 + 6x^{14}y^3 + \\
& 42480y^4 + 271440xy^4 + 804120x^2y^4 + 1491600x^3y^4 + 1966575x^4y^4 + 1947015x^5y^4 + \\
& 1453425x^6y^4 + 795285x^7y^4 + 306705x^8y^4 + 80745x^9y^4 + 14415x^{10}y^4 + 1755x^{11}y^4 + \\
& 120x^{12}y^4 + 84768y^5 + 478176xy^5 + 1246224x^2y^5 + 2014752x^3y^5 + 2256882x^4y^5 + \\
& 1810626x^5y^5 + 1029534x^6y^5 + 404694x^7y^5 + 108270x^8y^5 + 19470x^9y^5 + 2130x^{10}y^5 + \\
& 90x^{11}y^5 + 133392y^6 + 658272xy^6 + 1485792x^2y^6 + 2032572x^3y^6 + 1845207x^4y^6 + \\
& 1131927x^5y^6 + 466185x^6y^6 + 128745x^7y^6 + 23325x^8y^6 + 2565x^9y^6 + 195x^{10}y^6 + \\
& 15x^{11}y^6 + 169056y^7 + 718896xy^7 + 1368696x^2y^7 + 1518276x^3y^7 + 1057056x^4y^7 + \\
& 471300x^5y^7 + 136980x^6y^7 + 25560x^7y^7 + 3060x^8y^7 + 240x^9y^7 + 174252y^8 + \\
& 623472xy^8 + 963567x^2y^8 + 822057x^3y^8 + 415857x^4y^8 + 130635x^5y^8 + 25740x^6y^8 + \\
& 3240x^7y^8 + 180x^8y^8 + 146080y^9 + 424840xy^9 + 506860x^2y^9 + 313680x^3y^9 + \\
& 110820x^4y^9 + 23760x^5y^9 + 3020x^6y^9 + 200x^7y^9 + 20x^8y^9 + 98736y^{10} + \\
& 222714xy^{10} + 192828x^2y^{10} + 81990x^3y^{10} + 19830x^4y^{10} + 2610x^5y^{10} + 240x^6y^{10} + \\
& 52896y^{11} + 86970xy^{11} + 50850x^2y^{11} + 14460x^3y^{11} + 2220x^4y^{11} + 180x^5y^{11} + \\
& 21880y^{12} + 24100xy^{12} + 8875x^2y^{12} + 1725x^3y^{12} + 105x^4y^{12} + 15x^5y^{12} + 6720y^{13} + \\
& 4380xy^{13} + 1020x^2y^{13} + 120x^3y^{13} + 1440y^{14} + 450xy^{14} + 90x^2y^{14} + 192y^{15} + \\
& 18xy^{15} + 6x^2y^{15} + 12y^{16}).
\end{aligned}$$



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