The Tutte Polynomial of Phenylene Systems with Given Number of Branching Hexagons

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Abstract

Polynomial graph invariants have been confirmed to have important applications in quantum chemistry and biological information. One of the famous polynomial graph invariants is the Tutte polynomial which gives multifarious interesting information about the graph structure. In this paper, we first give a simpler and more efficient method to get the Tutte polynomials of alternating polycyclic chains. Then we obtain the explicit expressions for the Tutte polynomials and the number of spanning trees of phenylene systems with given number of branching hexagons. Moreover, we determine the extremal values of the number of spanning trees among the phenylene systems with given one or two branching hexagons, and the corresponding extremal phenylene systems are characterized, respectively.

Keywords: Tutte polynomial, phenylene system, spanning tree.

1 Introduction

Let $G = (V(G), E(G))$ be a graph with a finite vertex set $V(G)$ and a finite edge set $E(G)$. Let $G - e$ and G/e denote the graphs obtained from G by deleting and contracting the edge e, respectively. The Tutte polynomial, introduced by Tutte [17] in 1954 as a generalization of the chromatic polynomial, can be defined by the following deletion and contraction reduction formula.

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

It is generally known that the Tutte polynomial contains various interesting information about the structure and properties of graphs. If $x, y \in \{0, 1, 2\}$, then one can use $T(G; x, y)$ to get the number of certain graph invariant of graph G. For example, (i) $T(G; 1, 0)$ equals to the number of acyclic root-connected orientations of G; (ii) $T(G; 1, 1) = t(G)$,

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i.e., the number of spanning trees of G; (iii) $T(G;1,2)$ equals to the number of spanning connected subgraphs of G; (iv) $T(G;2,0)$ equals to the number of acyclic orientations of G; (v) $T(G;2,1)$ equals to the number of forests of G.

Although the Tutte polynomial have found various interesting applications in organic chemistry, biology and statistic physics [2], computing the Tutte polynomial of a graph is still a very challenging issue. In the general case, it is #P-hard for computing the Tutte polynomial of a graph [14, 15]. Thus, many work in this area is just focused on exploiting the structure of some specific classes of important graphs in order to derive closed-form formulas for computing their Tutte polynomials. In the recent years, the Tutte polynomials of some classes of chemical polycyclic graphs have been studied. Fath-Tabar, Gholam-Rezaei and Ashrafi [10] got the Tutte polynomial of benzenoid chains. Došlić [9] obtained the Tutte polynomials of several particular planar polycyclic graphs. Gong, Jin and Zhang [11] computed the Tutte polynomial of benzenoid systems with one branching hexagon by means of the relationship for Tutte polynomial of a graph and its dual graph. Dobrynin and Vesnin [6] given a general calculating scheme of polynomials based on deletion-contraction operations for uniform polycyclic chains. Chen and Guo [3] obtained the Tutte polynomials of some alternating polycyclic chains which contain phenylene chains as a special case. In [4], the author presented a splitting formula for the Tutte polynomial of a class of special compound graphs, and as an application the Tutte polynomials of catacondensed benzenoid systems with given number branching hexagons are also determined.

The phenylene system is known as a very important family of chemical molecular networks in which the carbon atoms form six-membered cycles and four-membered cycles. In particular, any two six-membered cycles (hexagons) are not adjacent, and every four-membered cycle (square) is adjacent to a pair of nonadjacent hexagons. If each hexagon of phenylene system is adjacent only to two squares, then the obtained chain is called the phenylene chain. If a hexagon in a phenylene system adjacent to three squares such that the three common edges are disjoint, then the hexagon will be named branching hexagon.

Nowadays, plenty of researches were focused on the phenylene system. The anti-Kekulé number and anti-forcing number of cata-condensed phenylenes are studied in [19] by Zhang, Bian and Vumar. Trantnik [16] characterized the extremal phenylene system with respect to the Wiener polarity index. A method for computing the edge-Wiener index and the edge-hyper-Wiener index of phenylenes is presented by Žigert [18], and the author further obtained closed formulas of the edge-Wiener index and the edge-hyper-Wiener index for linear phenylenes. The PI index for phenylene systems were studied in [8] and [12] respectively. Deng [7] talked about the phenylene systems with the third-order Randić index. Very recently, the first several extremal values of the Mostar indices for phenylene chains and tree-like phenylenes were obtained in [5] and [13].

In this paper, we mainly consider the Tutte polynomials for phenylene systems and determine the extremal values of the number of spanning trees for phenylene systems with given small number of branching hexagons.

2 Preliminaries

In this section, following the textbook on graph theory [1], we recall some basic known results and related properties linked to the enumeration of the Tutte polynomial.

Let C_r be a simple cycle with r vertices. Then the Tutte polynomial of C_r is given by

$$T(C_r; x, y) = y + \sum_{i=1}^{r-1} x^i = y - 1 + \frac{x^r - 1}{x - 1} = \frac{xy - x - y + x^r}{x - 1}.$$

Proposition 2.1 *Let $H \cdot F$ be the graph obtained from the union of two subgraphs H and F such that H and F share only a common vertex, then we have*

$$T(H \cdot F; x, y) = T(H; x, y)T(F; x, y).$$

And, if G contains s cut edges, t loops and no other edges, then we have $T(G; x, y) = x^s y^t$. Let G be a graph obtained from H by adding s cut edges and t loops, then

$$T(G; x, y) = x^s y^t T(H; x, y).$$

A planar graph is a graph that can be drawn on the plane so that their edges do not cross each other. Any such a drawing is called as a plane drawing. We use the abbreviation plane graph for a plane drawing of a planar graph. For a connected plane graph G, its dual graph $D(G)$ is a graph that has a vertex corresponding to each face of G, and an edge linking the vertices corresponding to neighboring faces for each edge of G. The following relation on the Tutte polynomial of a graph and its dual graph is well-known [1].

Proposition 2.2 *Let G be a connected plane graph and $D(G)$ the dual planar graph of G. Then it holds that $T(G;x,y) = T(D(G);y,x)$.*

Proposition 2.2 shows that if the dual graphs of two arbitrary plane graphs are isomorphic, then they possess the same Tutte polynomial.

The following splitting formula on Tutte polynomial is taken form [4].

Proposition 2.3 *Let $G|H$ be the graph obtained from G and H such that $E(G) \cup E(H) = E(G|H)$ and $E(G) \cap E(H) = \{e\}$, then*

$$T(G|H;x,y) = \frac{(xy-y-1)T_G T_H - y(x-1)(T_G T_{H-e} + T_{G-e} T_H) + xy T_{G-e} T_{H-e}}{xy-x-y}.$$

As a matter of convenience, some times we will use T_G or $T(G)$ in this article for the Tutte polynomial of a graph G and write $T(G;x,y)$ if we want to draw attention to the discussion.

3 The Tutte polynomials of alternating polycyclic chains

An alternating polycyclic chain is a graph formed by two types cycles C_r and C_s in which the induced C_rs and C_ss are arranged alternatively. Two adjacent cycles C_r and C_s in an alternating polycyclic chain share exactly an edge and each induced cycle of an alternating polycyclic chain has at most two common edges. Let $\mathcal{G}_n^{r,s}$ be the family of all alternating polycyclic chains with n copies of C_rs and $n-1$ copies of C_ss. Let $\mathcal{Z}_n^{r,s}$ be the family of alternating polycyclic chains with n copies of C_rs and n copies of C_ss. An arbitrary chain of $\mathcal{G}_n^{r,s}$ (resp. $\mathcal{Z}_n^{r,s}$) will be denoted by $G_n^{r,s}$ (resp. $Z_n^{r,s}$), i.e., $G_n^{r,s} \in \mathcal{G}_n^{r,s}$ and $Z_n^{r,s} \in \mathcal{Z}_n^{r,s}$. Some particular alternating polycyclic chains are shown in Figure 1.

Chen and Guo [3] obtained the Tutte polynomials of alternating polycyclic chains by applying a deletion-contraction-based scheme. In this section, we give a simper and more efficient method to get the Tutte polynomials of alternating polycyclic chains.

Lemma 3.1 *For any $G_n^{r,s}$ and $Z_n^{r,s}$, we have*

$$T(G_n^{r,s};x,y) = (y + \tfrac{x^{r-1}-1}{x-1})T(Z_{n-1}^{r,s};x,y) - x^{s-2}yT(G_{n-1}^{r,s};x,y), \tag{1}$$

$$T(Z_n^{r,s};x,y) = (y + \tfrac{x^{s-1}-1}{x-1})T(G_n^{r,s};x,y) - x^{r-2}yT(Z_{n-1}^{r,s};x,y). \tag{2}$$

Proof. We first note that an alternating polycyclic chain $G_n^{r,s}$ can be constructed by the way of $G_n^{r,s} = Z_{n-1}^{r,s}|C_r$ and let e be the common edge of the induced subgraphs $Z_{n-1}^{r,s}$ and C_r. It is not hard to get that $T(Z_{n-1}^{r,s} - e; x, y) = x^{s-2}T(G_{n-1}^{r,s}; x, y)$ and $T(C_r - e; x, y) = x^{r-1}$, then by the use of Proposition 2.3 we obtain (1). Similarly, one can see that $Z_n^{r,s} = G_n^{r,s}|C_s$ and assume that e' is the common edge of $G_n^{r,s}$ and C_s. Then we can easily obtain that $T(G_n^{r,s} - e'; x, y) = x^{r-2}T(Z_{n-1}^{r,s}; x, y)$ and $T(C_s - e'; x, y) = x^{s-1}$. Thus, by Proposition 2.3 and some basic simplifications we get (2). Therefore, we complete the proof. ∎

Lemma 3.2 *For any $G_n^{r,s}$ and $Z_n^{r,s}$, we have*

$$\begin{aligned} T(G_n^{r,s}; x, y) =& [(y + \tfrac{x^{s-1}-1}{x-1})(y + \tfrac{x^{r-1}-1}{x-1}) - y(x^{s-2} + x^{r-2})]T(G_{n-1}^{r,s}; x, y) \\ & - x^{r+s-4}y^2T(G_{n-2}^{r,s}; x, y), \end{aligned} \tag{3}$$

$$\begin{aligned} T(Z_n^{r,s}; x, y) =& [(y + \tfrac{x^{s-1}-1}{x-1})(y + \tfrac{x^{r-1}-1}{x-1}) - y(x^{s-2} + x^{r-2})]T(Z_{n-1}^{r,s}; x, y) \\ & - x^{r+s-4}y^2T(Z_{n-2}^{r,s}; x, y). \end{aligned} \tag{4}$$

Proof. For convenience we let $\varphi_1(x, y) = y + \frac{x^{r-1}-1}{x-1}$, $\varphi_2(x, y) = -x^{s-2}y$, $\psi_1(x, y) = y + \frac{x^{s-1}-1}{x-1}$ and $\psi_2(x, y) = -x^{r-2}y$. Then from (1) we have

$$T(Z_{n-1}^{r,s}; x, y) = \frac{1}{\varphi_1(x, y)}T(G_n^{r,s}; x, y) - \frac{\varphi_2(x, y)}{\varphi_1(x, y)}T(G_{n-1}^{r,s}; x, y) \tag{5}$$

and

$$T(Z_n^{r,s}; x, y) = \frac{1}{\varphi_1(x, y)}T(G_{n+1}^{r,s}; x, y) - \frac{\varphi_2(x, y)}{\varphi_1(x, y)}T(G_n^{r,s}; x, y). \tag{6}$$

Plugging (5) and (6) into (2) we get

$$\begin{aligned} T(G_n^{r,s}; x, y) =& [\varphi_1(x, y)\psi_1(x, y) + \varphi_2(x, y) + \psi_2(x, y)]T(G_{n-1}^{r,s}; x, y) \\ & - \varphi_2(x, y)\psi_2(x, y)T(G_{n-2}^{r,s}; x, y) \\ =& [(y + \tfrac{x^{s-1}-1}{x-1})(y + \tfrac{x^{r-1}-1}{x-1}) - y(x^{s-2} + x^{r-2})]T(G_{n-1}^{r,s}; x, y) \\ & - x^{r+s-4}y^2T(G_{n-2}^{r,s}; x, y). \end{aligned}$$

On the other hand, in terms of (2) we have

$$T(G_n^{r,s}; x, y) = \frac{1}{\psi_1(x, y)}T(Z_n^{r,s}; x, y) - \frac{\psi_2(x, y)}{\psi_1(x, y)}T(Z_{n-1}^{r,s}; x, y) \tag{7}$$

and

$$T(G^{r,s}_{n-1};x,y)=\frac{1}{\psi_1(x,y)}T(Z^{r,s}_{n-1};x,y)-\frac{\psi_2(x,y)}{\psi_1(x,y)}T(Z^{r,s}_{n-2};x,y). \tag{8}$$

If we substitute (7) and (8) into (1), then we get

$$\begin{aligned}T(Z^{r,s}_{n};x,y)=&[\psi_1(x,y)\varphi_1(x,y)+\psi_2(x,y)+\varphi_2(x,y)]T(Z^{r,s}_{n-1};x,y)\\&-\psi_2(x,y)\varphi_2(x,y)T(Z^{r,s}_{n-2};x,y)\\=&[(y+\tfrac{x^{s-1}-1}{x-1})(y+\tfrac{x^{r-1}-1}{x-1})-y(x^{s-2}+x^{r-2})]T(Z^{r,s}_{n-1};x,y)\\&-x^{r+s-4}y^2T(Z^{r,s}_{n-2};x,y).\end{aligned}$$

Thus the proof is completed. ■

In order to make the calculations more convenient, we let $G^{r,s}_1=C_r$ and $Z^{r,s}_0=K_2$. Then we have $G^{r,s}_2=(C_r|C_s)|C_r$ and $Z^{r,s}_1=C_r|C_s$. It is easy to obtain the initial conditions:

$$T(G^{r,s}_1;x,y)=T(C_r;x,y)=\tfrac{xy-x-y+x^r}{x-1}, \tag{9}$$

$$T(G^{r,s}_2;x,y)=\tfrac{xy-x-y+x^{2r-2}}{x-1}+\tfrac{(x^{s-2}-1)(xy-x-y+x^r)^2}{(x-1)^3}+\tfrac{(1+y)(xy-x-y+x^{r-1})^2}{(x-1)^2}, \tag{10}$$

$$T(Z^{r,s}_0;x,y)=T(K_2;x,y)=x, \tag{11}$$

$$T(Z^{r,s}_1;x,y)=T(C_r|C_s;x,y)=\tfrac{xy-x-y+x^{r+s-2}}{x-1}+\tfrac{(xy-x-y+x^{r-1})(xy-x-y+x^{s-1})}{(x-1)^2}. \tag{12}$$

Therefore, by combining the characteristic equatrion of (3) and the initial condition (9) and (10), we can get an explicit expression of the Tutte polynomial of $G^{r,s}_n$.

Theorem 3.3 *For any alternating polycyclic chain $G^{r,s}_n\in\mathcal{G}^{r,s}_n$, we have*

$$T(G^{r,s}_n;x,y)=\frac{2\omega-\gamma(\alpha-\sqrt{\Delta})}{\Delta+\alpha\sqrt{\Delta}}\Big(\frac{\alpha+\sqrt{\Delta}}{2}\Big)^n+\frac{2\omega-\gamma(\alpha+\sqrt{\Delta})}{\Delta-\alpha\sqrt{\Delta}}\Big(\frac{\alpha-\sqrt{\Delta}}{2}\Big)^n,$$

where $\Delta=\Delta(x,y)=\alpha(x,y)^2+4\beta(x,y)$, $\alpha=\alpha(x,y)=(y+\tfrac{x^{s-1}-1}{x-1})(y+\tfrac{x^{r-1}-1}{x-1})-y(x^{s-2}+x^{r-2})$, $\beta=\beta(x,y)=-x^{r+s-4}y^2$, $\gamma=\gamma(x,y)=\tfrac{xy-x-y+x^r}{x-1}$ *and* $\omega=\omega(x,y)=\tfrac{xy-x-y+x^{2r-2}}{x-1}+\tfrac{(x^{s-2}-1)(xy-x-y+x^r)^2}{(x-1)^3}+\tfrac{(1+y)(xy-x-y+x^{r-1})^2}{(x-1)^2}$.

Analogously, combining the characteristic equatrion of (4) and the initial condition (11) and (12), the Tutte polynomial of $Z^{r,s}_n$ can also be obtained.

Theorem 3.4 *For any alternating polycyclic chain $Z^{r,s}_n\in\mathcal{Z}^{r,s}_n$, we have*

$$T(Z^{r,s}_n;x,y)=\frac{2\eta-x(\alpha-\sqrt{\Delta})}{\Delta+\alpha\sqrt{\Delta}}\Big(\frac{\alpha+\sqrt{\Delta}}{2}\Big)^{n+1}+\frac{2\eta-x(\alpha+\sqrt{\Delta})}{\Delta-\alpha\sqrt{\Delta}}\Big(\frac{\alpha-\sqrt{\Delta}}{2}\Big)^{n+1},$$

where $\Delta = \alpha(x,y)^2 + 4\beta(x,y)$, $\alpha = \alpha(x,y) = (y + \frac{x^{s-1}-1}{x-1})(y + \frac{x^{r-1}-1}{x-1}) - y(x^{s-2} + x^{r-2})$, $\beta = \beta(x,y) = -x^{r+s-4}y^2$ *and* $\eta = \eta(x,y) = \frac{xy-x-y+x^{r+s-2}}{x-1} + \frac{(xy-x-y+x^{r-1})(xy-x-y+x^{s-1})}{(x-1)^2}$.

If we set $r = 6$, $s = 4$ in $\mathcal{G}_n^{r,s}$, then it is clearly that $\mathcal{G}_n^{6,4}$ contains all the molecular graphs of phenylene chains with n hexagons and $n-1$ squares. In the following we use PH_n to denote a phenylene chain with n hexagons and $n-1$ squares, i.e., $PH_n \in \mathcal{G}_n^{6,4}$. Thus, by theorem 3.4, we have the following result.

Corollary 3.5 *[3] Let PH_n be a phenylene chain with n hexagons and $n-1$ squares, then the Tutte polynomial of PH_n is given by*

$$T(PH_n; x, y) = \frac{2\omega - \gamma(\alpha - \sqrt{\Delta})}{\Delta + \alpha\sqrt{\Delta}}\Big(\frac{\alpha + \sqrt{\Delta}}{2}\Big)^n + \frac{2\omega - \gamma(\alpha + \sqrt{\Delta})}{\Delta - \alpha\sqrt{\Delta}}\Big(\frac{\alpha - \sqrt{\Delta}}{2}\Big)^n,$$

where $\Delta = \alpha^2 + 4\beta$, $\alpha = x^6 + 2x^5 + 3x^4 + x^3y + 3x^3 + x^2y + 3x^2 + 2xy + 2x + y^2 + 2y + 1, \beta = -x^6y^2$, $\gamma = y + x + x^2 + x^3 + x^4 + x^5$ *and* $\omega = x^{11} + 3x^{10} + 6x^9 + x^8y + 9x^8 + 2x^7y + 12x^7 + 5x^6y + 13x^6 + 8x^5y + 12x^5 + 2x^4y^2 + 9x^4y + 9x^4 + 2x^3y^2 + 8x^3y + 6x^3 + 2x^2y^2 + 7x^2y + 3x^2 + 3xy^2 + 4xy + x + y^3 + 2y^2 + y$.

Let $t(G) = T(G; 1, 1)$ be the number of spanning trees of a graph G. Then by Corollary 3.5, we get the number of spanning trees of PH_n.

Corollary 3.6 *[3] Let PH_n be a phenylene chain with n hexagons and $n-1$ squares, then the number of spanning trees of PH_n is given by*

$$t(PH_n) = \frac{(33 + 6\sqrt{30})(11 + 2\sqrt{30})^n}{120 + 22\sqrt{30}} + \frac{(33 - 6\sqrt{30})(11 - 2\sqrt{30})^n}{120 - 22\sqrt{30}}.$$

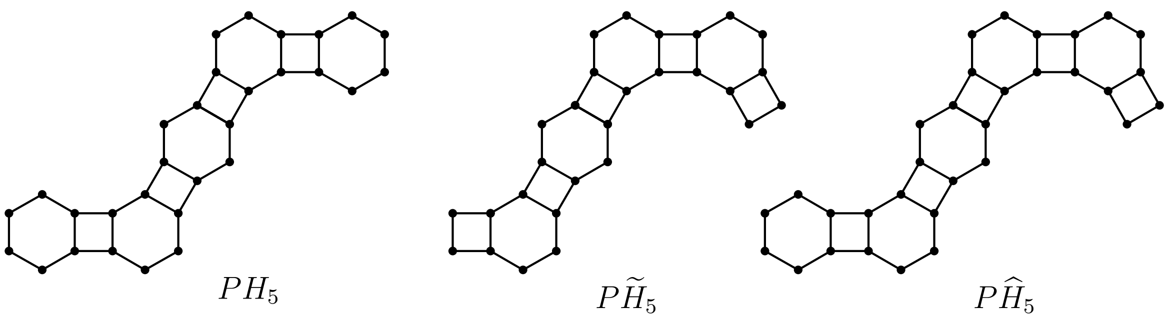

Figure 1. Some particular (modificatory) phenylene chains PH_5, $P\widetilde{H}_5$ and $P\widehat{H}_5$.

Setting $r = 4$, $s = 6$ in $\mathcal{G}_n^{r,s}$, then $\mathcal{G}_n^{4,6}$ contains all the molecular graphs of the modificatory phenylene chains with $n-1$ hexagons and n squares. We let $P\widetilde{H}_n$ be the modificatory phenylene chain with $n-1$ hexagons and n squares, i.e., $P\widetilde{H}_n \in \mathcal{G}_n^{4,6}$. Thus, by theorem 3.4, we have the following result.

Corollary 3.7 *[3] Let $P\widetilde{H}_n$ be a modificatory phenylene chain with $n-1$ hexagons and n squares. Then*

$$T(P\widetilde{H}_n; x, y) = \frac{2\omega - \gamma(\alpha - \sqrt{\Delta})}{\Delta + \alpha\sqrt{\Delta}}\Big(\frac{\alpha + \sqrt{\Delta}}{2}\Big)^n + \frac{2\omega - \gamma(\alpha + \sqrt{\Delta})}{\Delta - \alpha\sqrt{\Delta}}\Big(\frac{\alpha - \sqrt{\Delta}}{2}\Big)^n,$$

where $\Delta = \alpha^2 + 4\beta$, $\alpha = x^6 + 2x^5 + 3x^4 + x^3y + 3x^3 + x^2y + 3x^2 + 2xy + 2x + y^2 + 2y + 1$, $\beta = -x^6y^2$, $\gamma = y + x + x^2 + x^3$, $\omega = x^9 + 3x^8 + 6x^7 + 2x^6y + 8x^6 + 4x^5y + 9x^5 + 7x^4y + 8x^4 + x^3y^2 + 8x^3y + 6x^3 + 3x^2y^2 + 7x^2y + 3x^2 + 3xy^2 + 4xy + x + y^3 + 2y^2 + y$.

Since $t(P\widetilde{H}_n) = T(P\widetilde{H}_n; 1, 1)$, then by Corollary 3.7 we can get $t(P\widetilde{H}_n)$.

Corollary 3.8 *[3] The number of spanning trees of $P\widetilde{H}_n$ is given by*

$$t(P\widetilde{H}_n) = \frac{(22 + 4\sqrt{30})(11 + 2\sqrt{30})^n}{120 + 22\sqrt{30}} + \frac{(22 - 4\sqrt{30})(11 - 2\sqrt{30})^n}{120 - 22\sqrt{30}}.$$

By setting $r = 6$ and $s = 4$ in $\mathcal{Z}_n^{r,s}$, then $\mathcal{Z}_n^{6,4}$ contains all the modificatory phenylene chains (phenylene derivatives) with n hexagons and n squares. See Figure 1 for some particular (modificatory) phenylene chains.

By Theorem 3.4, we have the following result.

Corollary 3.9 *Let $P\widehat{H}_n$ be a modificatory phenylene chain with n hexagons and n squares, then we have*

$$T(P\widehat{H}_n; x, y) = \frac{2\eta - x(\alpha - \sqrt{\Delta})}{\Delta + \alpha\sqrt{\Delta}}\Big(\frac{\alpha + \sqrt{\Delta}}{2}\Big)^n + \frac{2\eta - x(\alpha + \sqrt{\Delta})}{\Delta - \alpha\sqrt{\Delta}}\Big(\frac{\alpha - \sqrt{\Delta}}{2}\Big)^n,$$

where $\Delta = \alpha^2 + 4\beta$, $\alpha = x^6 + 2x^5 + 3x^4 + x^3y + 3x^3 + x^2y + 3x^2 + 2xy + 2x + y^2 + 2y + 1$, $\beta = -x^6y^2$ *and* $\eta = x^7 + 2x^6 + 3x^5 + x^4y + 3x^4 + x^3y + 3x^3 + 2x^2y + 2x^2 + 2xy + x + y^2 + y$.

Therefore, by Corollary 3.9 we can get the number of spanning trees of $P\widehat{H}_n$.

Corollary 3.10 *The number of spanning trees of $P\widehat{H}_n$ is given by*

$$t(P\widehat{H}_n) = \frac{(6 + \sqrt{30})(11 + 2\sqrt{30})^{n+1}}{120 + 22\sqrt{30}} + \frac{(6 - \sqrt{30})(11 - 2\sqrt{30})^{n+1}}{120 - 22\sqrt{30}}.$$

4 The Tutte polynomial of phenylene systems with exactly one branching hexagon

A hexagon in a phenylene system is called branching hexagon if the induced hexagon has three pair-wise disjoint common edges with different squares. Let $PS_{l,m,n}$ be a phenylene

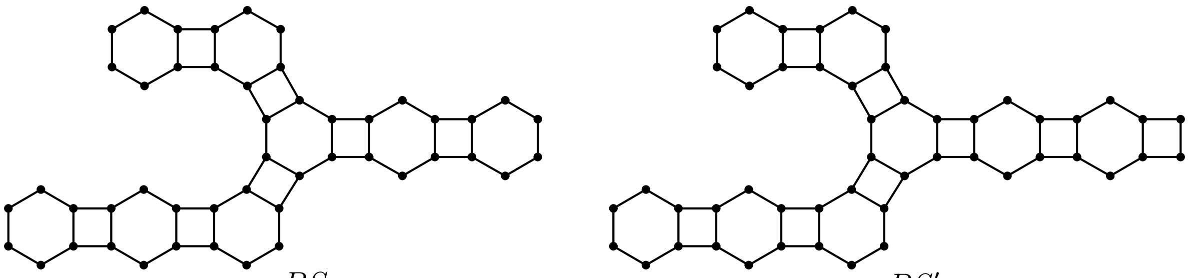

Figure 2. Two particular (decorated) phenylene systems $PS_{2,3,2}$ and $PS'_{2,3,2}$.

system with one branching hexagon and the three phenylene induced sub-chains of the phenylene system meeting at the branching hexagon have number of hexagons l, m and n respectively. A particular phenylene system $PS_{2,3,2}$ is shown in Figure 2.

As a matter of convenience, we will denote $T(PH_n; x, y)$ by T_n, denote $T(P\widetilde{H}_n; x, y)$ by $\widetilde{T}_n$, denote $T(P\widehat{H}_n; x, y)$ by $\widehat{T}_n$ and denote $T(PS_{l,m,n}; x, y)$ by $T_{l,m,n}$, respectively.

Theorem 4.1 *The Tutte polynomial of a phenylene system $PS_{l,m,n}$ can be given by*

$$T_{l,m,n} = \frac{(xy-y-1)T_{l+m+1}\widehat{T}_n - x^2y(x-1)T_{l+m+1}T_n - x^3y(x-1)\widehat{T}_l\widehat{T}_m\widehat{T}_n + x^6y\widehat{T}_l\widehat{T}_mT_n}{xy-x-y}.$$

Proof. We find that the graph $PS_{l,m,n}$ can be constructed by the way of that $PS_{l,m,n} = PH_{l+m+1}|P\widehat{H}_n$. If e is the common edge of PH_{l+m+1} and $P\widehat{H}_n$, then it is not difficult to obtain that $T(PH_{l+m+1} - e; x, y) = x^3T(P\widehat{H}_l; x, y)T(P\widehat{H}_m; x, y)$ and $T(P\widehat{H}_n - e; x, y) = x^2T(PH_n; x, y)$. Thus, by Proposition 2.3, we immediately get the desired result. ■

In addition, we also find that the phenylene system $PS_{l,m,n}$ can be constructed by the ways of $PS_{l,m,n} = PH_{l+n+1}|Z_m$ and $PS_{l,m,n} = PH_{m+n+1}|Z_l$, then similarly the Tutte polynomial of $PS_{l,m,n}$ can be given by

$$T_{l,m,n} = \frac{(xy-y-1)T_{l+n+1}\widehat{T}_m - x^2y(x-1)T_{l+n+1}T_m - x^3y(x-1)\widehat{T}_l\widehat{T}_n\widehat{T}_m + x^6y\widehat{T}_l\widehat{T}_nT_m}{xy-x-y}$$

and

$$T_{l,m,n} = \frac{(xy-y-1)T_{m+n+1}\widehat{T}_l - x^2y(x-1)T_{n+m+1}T_l - x^3y(x-1)\widehat{T}_n\widehat{T}_m\widehat{T}_l + x^6y\widehat{T}_n\widehat{T}_mT_l}{xy-x-y},$$

respectively.

Corollary 4.2 *The number of spanning trees of $PS_{l,m,n}$ can be given by*

$$t(PS_{l,m,n}) = t(PH_{l+m+1})t(P\widehat{H}_n) - t(P\widehat{H}_l)t(P\widehat{H}_m)t(PH_n). \tag{13}$$

Analogously, the number of spanning trees of $PS_{l,m,n}$ can also be expressed as

$$t(PS_{l,m,n}) = t(PH_{l+n+1})t(P\widehat{H}_m) - t(P\widehat{H}_l)t(P\widehat{H}_n)t(PH_m) \tag{14}$$

and

$$t(PS_{l,m,n}) = t(PH_{m+n+1})t(P\widehat{H}_l) - t(P\widehat{H}_m)t(P\widehat{H}_n)t(PH_l), \tag{15}$$

respectively.

In the subsequent discussion, we let $p = 11 + 2\sqrt{30}$, $q = 11 - 2\sqrt{30}$, $A = \frac{6+\sqrt{30}}{120+22\sqrt{30}}$, $B = \frac{6-\sqrt{30}}{120-22\sqrt{30}}$, $C = \frac{22+4\sqrt{30}}{120+22\sqrt{30}}$, $D = \frac{22-4\sqrt{30}}{120-22\sqrt{30}}$, $J = \frac{33+6\sqrt{30}}{120+22\sqrt{30}}$ and $Q = \frac{33-6\sqrt{30}}{120-22\sqrt{30}}$, then it is easy to see that $p-q = 4\sqrt{30} > 0$, $AB < 0$, $t(P\widehat{H}_n) = Ap^{n+1}+Bq^{n+1}$, $t(P\widetilde{H}_n) = Cp^n+Dq^n$ and $t(PH_n) = Jp^n + Qq^n$.

Let $\mathcal{PS}_{1,h}$ be the set of all phenylene systems with h hexagons in which there is exactly one branching hexagon. Next, we consider the extremal values of the number of spanning trees among all phenylene systems with one branching hexagon.

Lemma 4.3 *Let $PS_{l,m,n} \in \mathcal{PS}_{1,h}$, where $l + m + n = h - 1$. Without loss of generality we may assume that $l \le m \le n$.* (i) *If $l \ge 2$, then we have $t(PS_{l-1,m,n+1}) > t(PS_{l,m,n})$.* (ii) *If $m \ge 2$, then we have $t(PS_{l,m-1,n+1}) > t(PS_{l,m,n})$.* (iii) *If $l + 2 \le m$, then we have $t(PS_{l+1,m-1,n}) < t(PS_{l,m,n})$.* (iv) *If $l + 2 \le n$, then we have $t(PS_{l+1,m,n-1}) < t(PS_{l,m,n})$.*

Proof. (i) If $l \ge 2$, then by (14) we have

$$t(PS_{l-1,m,n+1}) = t(PH_{l+n+1})t(P\widehat{H}_m) - t(P\widehat{H}_{l-1})t(P\widehat{H}_{n+1})t(PH_m). \tag{16}$$

From (16) and (14), we get

$$\begin{aligned}
t(PS_{l-1,m,n+1}) - t(PS_{l,m,n}) =& t(PH_m)[t(P\widehat{H}_l)t(P\widehat{H}_n) - t(P\widehat{H}_{l-1})t(P\widehat{H}_{n+1})] \\
=& t(PH_m)AB[p^{l+1}q^{n+1} + p^{n+1}q^{l+1} - p^lq^{n+2} - p^{n+2}q^l] \\
=& t(PH_m)AB[p^lq^{n+1}(p-q) + p^{n+1}q^l(q-p)] \\
=& t(PH_m)AB(p-q)p^lq^l(q^{n-l+1} - p^{n-l+1}) \\
>& 0,
\end{aligned}$$

which means that $t(PH_{l-1,m,n+1}) > t(PH_{l,m,n})$.

(ii) If $m \ge 2$, then by (15) we have

$$t(PS_{l,m-1,n+1}) = t(PH_{l+n+1})t(P\widehat{H}_l) - t(P\widehat{H}_{m-1})t(P\widehat{H}_{n+1})t(PH_l).$$

Then we can get that

$$\begin{aligned}
t(PS_{l,m-1,n+1}) - t(PS_{l,m,n}) =& t(PH_l)[t(P\widehat{H}_m)t(P\widehat{H}_n) - t(P\widehat{H}_{m-1})t(P\widehat{H}_{n+1})] \\
=& t(PH_l)AB[p^{m+1}q^{n+1} + p^{n+1}q^{m+1} - p^m q^{n+2} - p^{n+2}q^m] \\
=& t(PH_l)AB[p^m q^{n+1}(p-q) + p^{n+1}q^m(q-p)] \\
=& t(PH_l)AB(p-q)p^m q^m(q^{n-m+1} - p^{n-m+1}) \\
>& 0,
\end{aligned}$$

which means $t(PS_{l,m-1,n+1}) > t(PS_{l,m,n})$.

(iii) If $l+2 \leq m$, then by (13) we can get

$$t(PS_{l+1,m,n-1}) = t(PH_{l+m+1})t(P\widehat{H}_n) - t(P\widehat{H}_{l+1})t(P\widehat{H}_{m-1})t(PH_n)$$

and

$$\begin{aligned}
t(PS_{l+1,m-1,n}) - t(PS_{l,m,n}) =& t(PH_n)[t(P\widehat{H}_l)t(P\widehat{H}_m) - t(P\widehat{H}_{l+1})t(P\widehat{H}_{m-1})] \\
=& t(PH_n)AB[p^l q^m + p^m q^l - p^{l+1}q^{m-1} - p^{m-1}q^{l+1}] \\
=& t(PH_n)AB[p^l q^{m-1}(q-p) + p^{m-1}q^l(p-q)] \\
=& t(PH_n)AB(p-q)p^l q^l(p^{m-l-1} - q^{m-l-1}) \\
<& 0,
\end{aligned}$$

which means $t(PS_{l+1,m-1,n}) < t(PS_{l,m,n})$.

(iv) If $l+2 \leq n$, then by (14) we can get

$$t(PS_{l+1,m,n-1}) = t(PH_{l+n+1})t(P\widehat{H}_m) - t(P\widehat{H}_{l+1})t(P\widehat{H}_{n-1})t(PH_m)$$

and

$$\begin{aligned}
t(PS_{l+1,m,n-1}) - t(PS_{l,m,n}) =& t(PH_m)[t(P\widehat{H}_l)t(P\widehat{H}_n) - t(P\widehat{H}_{l+1})t(P\widehat{H}_{n-1})] \\
=& t(PH_m)[ABp^l q^n + ABp^n q^l - ABp^{l+1}q^{n-1} - ABp^{n-1}q^{l+1}] \\
=& t(PH_m)[ABp^l q^{n-1}(q-p) + ABp^{n-1}q^l(p-q)] \\
=& t(PH_m)AB(p-q)p^l q^l(p^{n-l-1} - q^{n-l-1}) \\
<& 0.
\end{aligned}$$

Thus, we get $t(PS_{l+1,m,n-1}) < t(PS_{l,m,n})$. ■

From Lemma 4.3 we immediately have the following result.

Theorem 4.4 *For any $PS_{l,m,n} \in \mathcal{PS}_{1,h}$, $l \leq m \leq n$ and $l + m + n = h - 1$, we have*

$$t(PS_{1,1,h-3}) \geq t(PS_{l,m,n}) \geq \begin{cases} t(PS_{\frac{h-1}{3},\frac{h-1}{3},\frac{h-1}{3}}), & \text{if } h-1 \equiv 0 \pmod 3; \\ t(PS_{\frac{h-2}{3},\frac{h-2}{3},\frac{h+1}{3}}), & \text{if } h-1 \equiv 1 \pmod 3; \\ t(PS_{\frac{h-3}{3},\frac{h}{3},\frac{h}{3}}), & \text{if } h-1 \equiv 2 \pmod 3. \end{cases}$$

In the following we further consider the Tutte polynomial of a decorated phenylene system $PS'_{a,b,k}$ witch is obtained from $PS_{a,b,k}$ by joining a square to the pendent phenylene induced sub-chain having k hexagons. A decorated phenylene system $PS'_{2,3,2}$ is depicted in Figure 2.

Theorem 4.5 *Let $T'_{a,b,k} = T(PS'_{a,b,k}; x, y)$. Then we have that*

$$T'_{a,b,k} = \frac{[(xy - y - 1)T_{a+b+1} + y(x-1)x^3\widehat{T}_a\widehat{T}_b]\widetilde{T}_{k+1} - [yx^2(x-1)T_{a+b+1} - x^6y\widehat{T}_a\widehat{T}_b]\widehat{T}_k}{xy - x - y}.$$

Proof. According the structure of the decorated phenylene system $PS'_{a,b,k}$, we find it can be constructed by the way of that $PS'_{a,b,k} = PH_{a+b+1}|P\widetilde{H}_{k+1}$. If e is the common edge of the induced PH_{a+b+1} and $P\widetilde{H}_{k+1}$, then it can be got that $T(PH_{a+b+1} - e; x, y) = x^3T(P\widehat{H}_a; x, y)T(P\widehat{H}_b; x, y)$ and $T(P\widetilde{H}_{k+1} - e; x, y) = x^2T(P\widehat{H}_k; x, y)$. Thus, the desired result can be obtained by applying Proposition 2.3. ■

By Theorem 4.5 and $t(PS'_{a,b,k}) = T(PS'_{a,b,k}; 1, 1)$, we have

Corollary 4.6 *The number of spanning trees of $PS'_{a,b,k}$ can be given by*

$$t(PS'_{a,b,k}) = t(PH_{a+b+1})t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_a)t(P\widehat{H}_b)t(P\widehat{H}_k).$$

5 The Tutte polynomial of phenylene systems with exactly two branching hexagons

Let $PS^k_{a,b;c,d}$ be a phenylene system with exactly two branching hexagons in which one branching hexagon attached by two pendent phenylene sub-chains $P\widehat{H}_a$ and $P\widehat{H}_b$ respectively, the other branching hexagon attached by two pendent phenylene sub-chains $P\widehat{H}_c$ and $P\widehat{H}_d$ respectively, and there is a phenylene sub-chain $P\widetilde{H}_{k+1}$ connecting the two branching hexagons. A particular phenylene system $PS^2_{2,3;4,3}$ is depicted in Figure 3. Obviously, if $k = 0$, then there is only a square between the two branching hexagons of $PS^0_{a,b;c,d}$.

If we consider the linking orientations of the four induced pendent sub-chains meeting at the two branching hexagons, $a \neq b$ and $c \neq d$, then $PS^k_{a,b;c,d} \ncong PS^k_{a,b;d,c}$. But they have the same Tutte polynomial, i.e., $T(PS^k_{a,b;c,d}; x, y) = T(PS^k_{a,b;d,c}; x, y)$, since the dual graphs of them are isomorphic. So, in the following we will use $PS^k_{a,b;c,d}$ to denote a graph taking from $\{PS^k_{a,b;c,d}, PS^k_{a,b;d,c}, PS^k_{b,a;c,d}, PS^k_{b,a;d,c}\}$, indiscriminatedly.

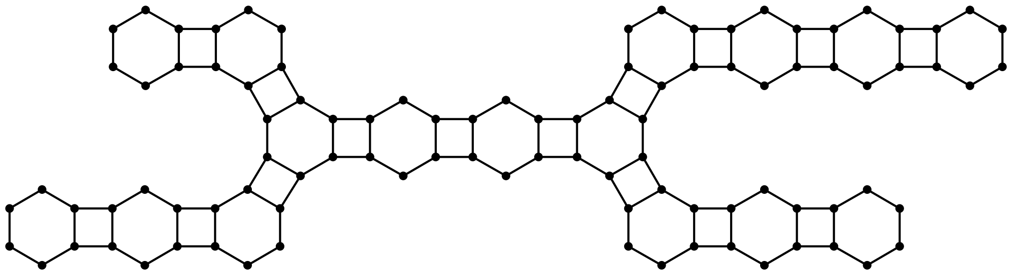

Figure 3. A phenylene system $PS^2_{2,3;4,3}$.

Theorem 5.1 *For the phenylene system $PS^0_{a,b;c,d}$, we have*

$$T(PS^0_{a,b;c,d}; x, y) = \phi_1 \cdot T_{a+b+1}T_{c+d+1} - \phi_2 \cdot (T_{a+b+1}\widehat{T}_c\widehat{T}_d + T_{c+d+1}\widehat{T}_a\widehat{T}_b) + \phi_3 \cdot \widehat{T}_a\widehat{T}_b\widehat{T}_c\widehat{T}_d,$$

where $\phi_1 = \frac{x^2y-x^2+xy^2-x-y^2-2y-1}{xy-x-y}$, $\phi_2 = \frac{x^3y(xy-y-1)}{xy-x-y}$ *and* $\phi_3 = \frac{x^6y^2(x-1)}{xy-x-y}$.

Proof. We can see that $PS^0_{a,b;c,d} = (PH_{a+b+1}|C_4)|PH_{c+d+1}$. Let e be the common edge of PH_{a+b+1} and C_4, then it is easy to get $T(PH_{a+b+1} - e; x, y) = x^3T(P\widehat{H}_a; x, y)T(P\widehat{H}_b; x, y)$ and $T(C_4 - e; x, y) = x^3$. Thus by Proposition 2.3 and some basic calculations we get

$$T(PH_{a+b+1}|C_4; x, y) = (x^2 + x + y + 1)T_{a+b+1} - x^3y\widehat{T}_a\widehat{T}_b. \tag{17}$$

Let e' be the common edge of $PH_{a+b+1}|C_4$ and PH_{c+d+1}. Then it is not difficultly to obtain that $T(PH_{a+b+1}|C_4 - e'; x, y) = x^2T(PH_{a+b+1}; x, y)$ and $T(PH_{c+d+1} - e'; x, y) = x^3T(P\widehat{H}_c; x, y)T(P\widehat{H}_d; x, y)$. Combining Proposition 2.3 and (17) one can obtain the required result. ■

By setting $x = y = 1$ in Theorem 5.1, we find that

Corollary 5.2 *The number of spanning trees of $PS^0_{a,b;c,d}$ is given by*

$$t(PS^0_{a,b;c,d}) = t(PH_{c+d+1})[4t(PH_{a+b+1}) - t(P\widehat{H}_a)t(P\widehat{H}_b)] - t(PH_{a+b+1})t(P\widehat{H}_c)t(P\widehat{H}_d).$$

Now, we consider the Tutte polynomial of $PS^k_{a,b;c,d}$ with $k \geq 1$.

Theorem 5.3 *For the phenylene system $PS^k_{a,b;c,d}$, $k \geq 1$, we have*

$$T(PS^k_{a,b;c,d}) = \frac{[(xy-y-1)\widehat{T}_d - x^2y(x-1)T_d]T_{a,b,k+c+1} + [x^6y\widehat{T}_cT_d - x^3y(x-1)\widehat{T}_c]T'_{a,b,k}}{xy-x-y}.$$

Proof. We first note that $PS^k_{a,b;c,d} = PS_{a,b,k+c+1}|P\widehat{H}_d$ and let e be the common edge of the induced subgraphs $PS_{a,b,k+c+1}$ and $P\widehat{H}_d$. And we can get $T(PS_{a,b,k+c+1} - e; x, y) = x^3T(PS'_{a,b,k}; x, y)\widehat{T}_c$ and $T(P\widehat{H}_d - e; x, y) = x^2T(PH_d; x, y)$. Thus, by applying Proposition 2.3 we obtain the required result. ■

Corollary 5.4 *The number of spanning trees of $PS^k_{a,b;c,d}$ is given by*

$$t(PS^k_{a,b;c,d}) = t(P\widehat{H}_d)t(PS_{a,b,k+c+1}) - t(P\widehat{H}_c)t(PH_d)t(PS'_{a,b,k}).$$

From Corollary 4.6 and Corollary 5.4, the number of spanning tees of $PS^k_{a,b;c,d}$ can also be written as $t(PS^k_{a,b;c,d}) = t(P\widehat{H}_d)[t(PH_{a+b+1})t(P\widehat{H}_{k+c+1}) - t(P\widehat{H}_a)t(P\widehat{H}_b)t(PH_{k+c+1})] - t(P\widehat{H}_c)t(PH_d)[t(PH_{a+b+1})t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_a)t(P\widehat{H}_b)t(P\widehat{H}_c)]$.

Let $\mathcal{PS}_{2,h}$ be the set of all phenylene systems with h hexagons in which there is exactly two branching hexagons. The next we consider the extremal values of the number of spanning trees among $\mathcal{PS}_{2,h}$.

Lemma 5.5 *Let $PS^k_{a,b;c,d} \in \mathcal{PS}_{2,h}$, where $a+b+c+d+k+2 = h$.* (i) *If $a \geq 2$, then it holds that $t(PS^{k+1}_{a-1,b;c,d}) > t(PS^k_{a,b;c,d})$.* (ii) *If $b \geq 2$, then it holds that $t(PS^{k+1}_{a,b-1;c,d}) > t(PS^k_{a,b;c,d})$.* (iii) *If $c \geq 2$, then it holds that $t(PS^{k+1}_{a,b;c-1,d}) > t(PS^k_{a,b;c,d})$.* (iv) *If $d \geq 2$, then it holds that $t(PS^{k+1}_{a,b;c,d-1}) > t(PS^k_{a,b;c,d})$.*

Proof. Here we just give the proof of (iii) since the statements (i), (ii) and (iv) can be proved by a similar way. Bearing in mind that $A = \frac{6+\sqrt{30}}{120+22\sqrt{30}}$ and $B = \frac{6-\sqrt{30}}{120-22\sqrt{30}}$ and let $C = \frac{22+4\sqrt{30}}{120+22\sqrt{30}} > 0$, $D = \frac{22-4\sqrt{30}}{120-22\sqrt{30}} < 0$, then we can get

$$\begin{aligned} t(P\widehat{H}_c)t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_{c-1})t(P\widetilde{H}_{k+2}) =& (Ap^{c+1} + Bq^{c+1})(Cp^{k+1} + Dq^{k+1}) \\ & - (Ap^c + Bq^c)(Cp^{k+2} + Dq^{k+2}) \\ =& AD(p^{c+1}q^{k+1} - p^cq^{k+2}) + BC(p^{k+1}q^{c+1} - p^{k+2}q^c) \end{aligned}$$

and

$$t(P\widehat{H}_{c-1})t(P\widehat{H}_{k+1}) - t(P\widehat{H}_c)t(P\widehat{H}_k) = (Ap^c + Bq^c)(Cp^{k+2} + Dq^{k+2})$$

$$
\begin{aligned}
&- (Ap^{c+1} + Bq^{c+1})(Cp^{k+1} + Dq^{k+1}) \\
=&AB(q-p)(p^c q^{k+1} - p^{k+1} q^c).
\end{aligned}
$$

Case 1. $c \geq 2$ and $k = c-1$. In this case, we first can show that

$$
\begin{aligned}
t(P\widehat{H}_c)t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_{c-1})t(P\widetilde{H}_{k+2}) =&AD(p^{c+1}q^{k+1} - p^c q^{k+2}) + BC(p^{k+1}q^{c+1} - p^{k+2}q^c) \\
=&AD(p^{c+1}q^c - p^c q^{c+1}) + BC(p^c q^{c+1} - p^{c+1}q^c) \\
=&p^c q^c (p-q)(AD - BC) > 0
\end{aligned}
$$

and

$$
t(P\widehat{H}_{c-1})t(P\widehat{H}_{k+1}) - t(P\widehat{H}_c)t(P\widehat{H}_k) = AB(q-p)(p^c q^{k+1} - p^{k+1}q^c) = 0.
$$

So, we have

$$
\begin{aligned}
t(PS^{k+1}_{a,b;c-1,d}) - t(PS^k_{a,b;c,d}) =&t(P\widehat{H}_c)t(PH_d)t(PS'_{a,b,k}) - t(P\widehat{H}_{c-1})t(PH_d)t(PS'_{a,b,k+1}) \\
=&t(PH_d)[t(P\widehat{H}_c)t(PS'_{a,b,k}) - t(P\widehat{H}_{c-1})t(PS'_{a,b,k+1})] \\
=&t(PH_d)\big[t(PH_{a+b+1})\big(t(P\widehat{H}_c)t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_{c-1})t(P\widetilde{H}_{k+2})\big) \\
&+ t(P\widehat{H}_a)t(P\widehat{H}_b)\big(t(P\widehat{H}_{c-1})t(P\widehat{H}_{k+1}) - t(P\widehat{H}_c)t(P\widehat{H}_k)\big)\big] \\
=&p^c q^c (p-q)(AD - BC)t(PH_d)t(PH_{a+b+1}) > 0.
\end{aligned}
$$

Case 2. $c \geq 2$ and $k > c-1$. In this case, we have

$$
\begin{aligned}
t(P\widehat{H}_c)t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_{c-1})t(P\widetilde{H}_{k+2}) =&(Ap^{c+1} + Bq^{c+1})(Cp^{k+1} + Dq^{k+1}) \\
&- (Ap^c + Bq^c)(Cp^{k+2} + Dq^{k+2}) \\
=&AD(p^{c+1}q^{k+1} - p^c q^{k+2}) + BC(p^{k+1}q^{c+1} - p^{k+2}q^c) \\
=&ADp^c q^{k+1}(p-q) + BCp^{k+1}q^c(q-p) \\
=&p^c q^c (p-q)(q^{k-c+1}AD - p^{k-c+1}BC) > 0
\end{aligned}
$$

and

$$
\begin{aligned}
t(P\widehat{H}_{c-1})t(P\widehat{H}_{k+1}) - t(P\widehat{H}_c)t(P\widehat{H}_k) =&(Ap^c + Bq^c)(Ap^{k+2} + Bq^{k+2}) \\
&- (Ap^{c+1} + Bq^{c+1})(Ap^{k+1} + Bq^{k+1}) \\
=&AB(q-p)(p^c q^{k+1} - p^{k+1}q^c) \\
=&AB(q-p)p^c q^c (q^{k-c+1} - p^{k-c+1}) < 0.
\end{aligned}
$$

Note that $t(PH_d)t(PH_{a+b+1}) > t(PH_d)t(P\widehat{H}_a)t(P\widehat{H}_b)$, then we can obtain that

$$\begin{aligned}
t(PS^{k+1}_{a,b;c-1,d}) - t(PS^{k}_{a,b;c,d}) =& t(PH_d)t(PH_{a+b+1})[t(P\widehat{H}_c)t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_{c-1})t(P\widetilde{H}_{k+2})] \\
&+ t(PH_d)t(P\widehat{H}_a)t(P\widehat{H}_b)[t(P\widehat{H}_{c-1})t(P\widehat{H}_{k+1}) - t(P\widehat{H}_c)t(P\widehat{H}_k)] \\
>& t(P\widehat{H}_c)t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_{c-1})t(P\widetilde{H}_{k+2}) \\
&+ t(P\widehat{H}_{c-1})t(P\widehat{H}_{k+1}) - t(P\widehat{H}_c)t(P\widehat{H}_k) \\
=& t(P\widehat{H}_c)[t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_k)] \\
&+ t(P\widehat{H}_{c-1})[t(P\widehat{H}_{k+1}) - t(P\widetilde{H}_{k+2})] \\
=& (Ap^{c+1} + Bq^{c+1})(Cp^{k+1} + Dq^{k+1} - Ap^{k+1} - Bq^{k+1}) \\
&+ (Ap^{c} + Bq^{c+1})(Ap^{k+2} + Bq^{k+2} - Cp^{k+2} - Dq^{k+2}) \\
=& A(B-D)p^cq^{k+1}(q-p) + B(A-C)p^{k+1}q^c(p-q) \\
=& p^cq^c(p-q)[B(A-C)p^{k-c+1} - A(B-D)q^{k-c+1}] > 0.
\end{aligned}$$

Case 3. $c \geq 2$ and $k < c-1$. We have

$$\begin{aligned}
t(P\widehat{H}_c)t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_{c-1})t(P\widetilde{H}_{k+2}) =& ADp^cq^{k+1}(p-q) + BCp^{k+1}q^c(q-p) \\
=& p^{k+1}q^{k+1}(p-q)(q^{c-k-1}AD - p^{c-k-1}BC) > 0
\end{aligned}$$

and

$$\begin{aligned}
t(P\widehat{H}_{c-1})t(P\widehat{H}_{k+1}) - t(P\widehat{H}_c)t(P\widehat{H}_k) =& AB(q-p)(p^cq^{k+1} - p^{k+1}q^c) \\
=& AB(q-p)p^{k+1}q^{k+1}(q^{c-k-1} - p^{c-k-1}) < 0.
\end{aligned}$$

Since $t(PH_d)t(PH_{a+b+1}) > t(PH_d)t(P\widehat{H}_a)t(P\widehat{H}_b)$, then we have

$$\begin{aligned}
t(PS^{k+1}_{a,b;c-1,d}) - t(PS^{k}_{a,b;c,d}) =& t(PH_d)t(PH_{a+b+1})[t(P\widehat{H}_c)t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_{c-1})t(P\widetilde{H}_{k+2})] \\
&+ t(PH_d)t(P\widehat{H}_a)t(P\widehat{H}_b)[t(P\widehat{H}_{c-1})t(P\widehat{H}_{k+1}) - t(P\widehat{H}_c)t(P\widehat{H}_k)] \\
>& t(P\widehat{H}_c)t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_{c-1})t(P\widetilde{H}_{k+2}) \\
&+ t(P\widehat{H}_{c-1})t(P\widehat{H}_{k+1}) - t(P\widehat{H}_c)t(P\widehat{H}_k) \\
=& t(P\widehat{H}_c)[t(P\widetilde{H}_{k+1}) - t(P\widehat{H}_k)] \\
&+ t(P\widehat{H}_{c-1})[t(P\widehat{H}_{k+1}) - t(P\widetilde{H}_{k+2})] \\
=& A(B-D)p^cq^{k+1}(q-p) + B(A-C)p^{k+1}q^c(p-q) \\
=& p^{k+1}q^{k+1}(p-q)[B(A-C)p^{c-k-1} - A(B-D)q^{c-k-1}] > 0.
\end{aligned}$$

Therefore, we obtain that $t(PS^{k+1}_{a,b;c-1,d}) > t(PS^{k}_{a,b;c,d})$ for $c \geq 2$. ■

Lemma 5.6 *Let $PS^0_{a,b;c,d}$ be a phenylene system with two branching hexagons.* (i) *If $a \geq b+2$, then it holds that $t(PS^0_{a,b;c,d}) > t(PS^0_{a-1,b+1;c,d})$.* (ii) *If $b \geq a+2$, then it holds that $t(PS^0_{a,b;c,d}) > t(PS^0_{a+1,b-1;c,d})$.* (iii) *If $c \leq d+2$, then it holds that $t(PS^0_{a,b;c,d}) > t(PS^0_{a,b;c-1,d+1})$.* (iv) *If $d \leq c+2$, then it holds that $t(PS^0_{a,b;c,d}) > t(PS^0_{a,b;c+1,d-1})$.*

Proof. (i) The number of spanning trees of $PS^0_{a,b;c,d}$ and $PS^0_{a-1,b+1;c,d}$ can be respectively written as

$$\begin{aligned}t(PS^0_{a,b;c,d}) =& t(PH_{a+b+1})(t(P\widehat{H}_d)t(P\widehat{H}_{c+1}) - 4t(PH_d)t(P\widehat{H}_c))\\ &+ t(P\widehat{H}_a)t(P\widehat{H}_b)(t(P\widehat{H}_c) - t(PH_{c+1}))\end{aligned}$$

and

$$\begin{aligned}t(PS^0_{a-1,b+1;c,d}) =& t(PH_{a+b+1})(t(P\widehat{H}_d)t(P\widehat{H}_{c+1}) - 4t(PH_d)t(P\widehat{H}_c))\\ &+ t(P\widehat{H}_{a-1})t(P\widehat{H}_{b+1})(t(P\widehat{H}_c) - t(PH_{c+1})).\end{aligned}$$

Then we have

$$\begin{aligned}t(PS^0_{a-1,b+1;c,d}) - t(PS^0_{a,b;c,d}) =& (t(P\widehat{H}_c) - t(PH_{c+1}))[t(P\widehat{H}_{a-1})t(P\widehat{H}_{b+1}) - t(P\widehat{H}_a)t(P\widehat{H}_b)]\\ =& (t(P\widehat{H}_c) - t(PH_{c+1}))[(Cp^{a-1} + Dq^{a-1})(Cp^{b+1} + Dq^{b+1})\\ &- (Cp^a + Dq^a)(Cp^b + Dq^b)]\\ =& (t(P\widehat{H}_c) - t(PH_{c+1}))CD[(p^{a-1}q^{b+1} - p^aq^b)\\ &+ (p^{b+1}q^{a-1} - p^bq^a)]\\ =& (t(P\widehat{H}_c) - t(PH_{c+1}))CDp^bq^b(q^{a-b-1} - p^{a-b-1}) < 0.\end{aligned}$$

Thus, we get $t(PS^0_{a,b;c,d}) > t(PS^0_{a-1,b+1;c,d})$ for $a \geq b+2$. The statements (ii)-(iv) can be proved similarly, we omit the proof here. ∎

Lemma 5.7 *For the number of spanning trees of the phenylene systems $PS^0_{k,k+1;k,k+1}$ and $PS^0_{k+1,k+1;k,k}$, we have $t(PS^0_{k,k+1;k,k+1}) > t(PS^0_{k+1,k+1;k,k})$.*

Proof. From Corollary 5.2, we have

$$\begin{aligned}t(PS^0_{k,k+1;k,k+1}) =& 4t(PH_{2k+2})^2 - 2t(PH_{2k+2})t(P\widehat{H}_k)t(P\widehat{H}_{k+1}),\\ t(PS^0_{k+1,k+1;k,k}) =& 4t(PH_{2k+3})t(PH_{2k+1}) - t(PH_{2k+1})t(P\widehat{H}_{k+1})t(P\widehat{H}_{k+1})\end{aligned}$$

$$- t(PH_{2k+3})t(P\widehat{H}_k)t(P\widehat{H}_k).$$

Then, bearing in mind that $t(P\widehat{H}_n) = Ap^{n+1} + Bq^{n+1}$ and $t(PH_n) = Jp^n + Qq^n$, one can get

$$\begin{aligned} t(PS^0_{k,k+1;k,k+1}) - t(PS^0_{k,k;k+1,k+1}) =& p^{1+2k}(p-q)^2(B^2qJ + A^2pQ - 4JQ) \\ =& \tfrac{3}{10}p^{1+2k}(p-q)^2 > 0. \end{aligned}$$

Thus, we obtain the result $t(PS^0_{k,k+1;k,k+1}) > t(PS^0_{k+1,k+1;k,k})$. ■

From Lemma 5.5, Lemma 5.6 and Lemma 5.7 we immediately get the following result.

Theorem 5.8 *For $PS^k_{a,b;c,d} \in \mathcal{PS}_{2,h}$, where $a+b+c+d = h-k-2$, we have*

$$t(PS^{h-6}_{1,1;1,1}) \geq t(PS^k_{a,b;c,d}) \geq \begin{cases} t(PS^0_{\frac{h-2}{4},\frac{h-2}{4};\frac{h-2}{4},\frac{h-2}{4}}), & \text{if } h-2 \equiv 0 \pmod 4; \\ t(PS^0_{\frac{h-3}{4},\frac{h-3}{4};\frac{h-3}{4},\frac{h+1}{4}}), & \text{if } h-2 \equiv 1 \pmod 4; \\ t(PS^0_{\frac{h-4}{4},\frac{h-4}{4};\frac{h}{4},\frac{h}{4}}), & \text{if } h-2 \equiv 2 \pmod 4; \\ t(PS^0_{\frac{h-5}{4},\frac{h-1}{4};\frac{h-1}{4},\frac{h-1}{4}}), & \text{if } h-2 \equiv 3 \pmod 4. \end{cases}$$

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