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# *On the Tutte polynomial of benzenoid chains*

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## ABSTRACT

The Tutte polynomial of a graph G, T(G, x,y) is a polynomial in two variables defined for every undirected graph contains information about how the graph is connected. In this paper a simple formula for computing Tutte polynomial of a benzenoid chain is presented.

**Keywords**: Benzenoid chain, Tutte polynomial, graph.

## 1. INTRODUCTION

*Benzenoid graphs* or graph representations of benzenoid hydrocarbons are defined as finite connected plane graphs with no cut-vertices, in which all interior regions are mutually congruent regular hexagons. More details on this important class of molecular graphs can be found in the book of Gutman and Cyvin [1], and in the references cited therein.

Suppose $G$ is an undirected graph, $E = E(G)$ and $v$ is a vertex of $G$. The vertex $v$ is reachable from another vertex $u$ if there is a path in $G$ connecting u and v. In this case we write $v\alpha u$. A single vertex is a path of length zero and so $\alpha$ is reflexive. Moreover, we can easily prove that $\alpha$ is symmetric and transitive. So $\alpha$ is an equivalence relation on $V(G)$. The equivalence classes of $\alpha$ is called the *connected components* of $G$. The *Tutte polynomial* of a graph G is a polynomial in two variables defined for every undirected graph contains information about how the graph is connected [2-4]. To define we need some notions. The edge contraction G/uv of the graph G is the graph obtained by merging the vertices u and v and removing the edge uv. We write $G - uv$ for the graph where the edge $uv$ is merely removed. Then the Tutte polynomial of $G$ is defined by the recurrence relation $T[G; x, y) = T(G - e; x, y) + T(G/e; x, y)$ if $e$ is neither a loop nor a bridge with base case $T(G; x, y) = x^i y^j$ if $G$ contains $i$ bridges and $j$ loops and no other edges. In particular,

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T(*G; x, y*) = 1 if *G* contains no edges. The importance of the Tutte polynomial *T*(G, x, y) comes from the algebraic graph theory as a generalization of counting problems related to graph coloring and nowhere-zero flow. It is also the source of several central computational problems in theoretical computer science.

In this paper, the Tutte polynomial of a benzenoid chain BC($x_1$, ..., $x_r$) is computed. This graph is constructed from r linear chains of length $x_1$, $x_2$, …, $x_r$, respectively. Suppose BC(h) denotes the set of all benzenoid chains with h hexagons.


**Figure 1**. The Molecular Graph of a Linear Chain BC(h).

In Figures 1 and 2, the molecular graph of a linear chain LC(h) and BC(2,3,2,2,4,2,3,2,2) is depicted.

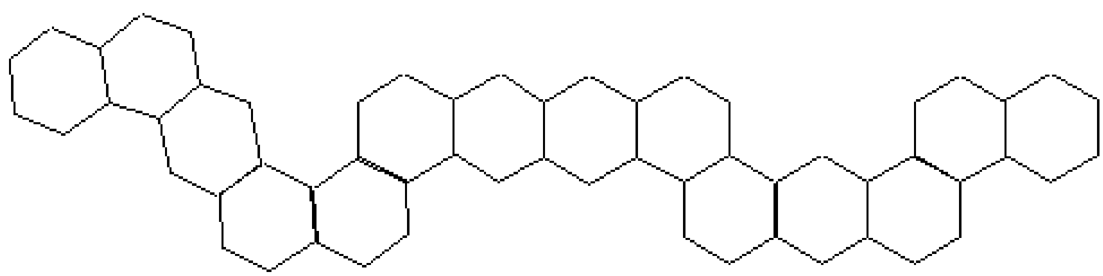

**Figure 2.** The Molecular Graph of a Benzenoid Chain BC(2,3,2,2,4,2,3,2,2).

Throughout this article our notation is standard and taken mainly from the standard book of graph theory.

## 2. MAIN RESULTS

In this section the Tutte polynomial of a benzenoid chain *G*(*h*) is computed. We first notice that, one can define the Tutte polynomial of a graph *G* as folice thlows:

$$T(G; x, y) = \Sigma_{A\subseteq E(G)} (x-1)^{c(A)-c(E)} (y-1)^{c(A)+|A|-|V|}.$$

Here, c($A$) denotes the number of connected components of the graph ($V$,$A$).

**Theorem 1.** $T(BC(x_1, x_2, \ldots, x_n); x, y) = T(LBC(x_1 + \ldots + x_n - n + 1); x, y)$.

**Proof**. We proceed by induction on n to prove

$$T(BC(x_1, x_2, \ldots, x_n); x, y) = T(LBC(x_1 + \ldots + x_n - n + 1); x, y),$$

and

$$T(BC(x_1, x_2, \ldots, x_n)\sim C_5; x, y) = T(LBC(x_1 + \ldots + x_n - n + 1)\sim C_5; x, y).$$

Clearly the result is valid for n = 1. Suppose the validity of result for n = k and prove it for n = k + 1. Our main proof consider two cases that $x_{k+1} = 2$ or $x_{k+1} > 2$. If $x_{k+1} = 2$ then

$$\begin{aligned} T(BC(x_1, x_2, \ldots, x_k,2); x, y) &= x^4T(BC(x_1, x_2, \ldots, x_k); x, y) + T(BC(x_1, x_2, \ldots, x_k)\sim C_5; x, y) \\ &= (x4 + x3 + x2 + x + 1)T(BC(x_1, x_2, \ldots, x_k); x, y) \\ &+ y\, T(BC(x_1, x_2, \ldots, x_{k-1},x_k-1)\sim C_5; x, y) \\ &= T(LBC(x_1 + \ldots + x_k - k + 2); x, y), \end{aligned}$$

as desired. On the other hand, by a similar method one can prove that

$$T(BC(x_1, x_2, \ldots, x_k,2)\sim C_5; x, y) = T(LBC(x_1 + \ldots + x_k - k + 2)\sim C_5; x, y).$$

We now assume that $m = x_{k+1} > 2$ and the result is valid for m. We have:

$$\begin{aligned} T(BC(x_1, x_2, \ldots, x_k,m+1); x, y) &= (x^4+x^3+x^2+x+1)\, T(BC(x_1, x_2, \ldots, x_k,m); x, y) \\ &+ yT(BC(x_1,\ldots,x_k,m)\sim C_5; x, y) \\ &= (x^4+x^3+x^2+x+1)\, T(LBC(x_1+ x_2+\ldots+ x_k+m-k ); x, y) \\ &+ yT(LBC(x_1+\ldots+x_k+m-k)\sim C_5; x, y), \end{aligned}$$

which completes our proof. □

Before stating the main result of this paper we notice that if h = 1, 2 then

$T(G(0), x,y)=x$, where G(0) is an edge,
$T(G(1), x, y) = x^5 + x^4 + x^3 + x^2 + x + y.$

**Theorem 2.** Suppose $G = G(x_1,x_2,\ldots,x_n)$ is an arbitrary benzenoid chain in BC(h), where $h = x_1 + x_2 + \ldots + x_n - n + 1$. Then for $h > 2$

$$T(G,x,y) = \left(\frac{x(J+\sqrt{\Delta})+2(1-x)y}{2\sqrt{\Delta}}\right)\left(\frac{J+\sqrt{\Delta}}{2}\right)^n + \left(\frac{x(-J+\sqrt{\Delta})-2(1-x)y)}{2\sqrt{\Delta}}\right)\left(\frac{J-\sqrt{\Delta}}{2}\right)^n,$$

where

$$J = x^4 + x^3 + x^2 + x + 1 + y,$$
$$\Delta = (x^4 + x^3 + x^2 + x + 1)^2 + y^2 + 2y(x^4 + x^3 + x^2 + x + 1) - 4x^4 y.$$

**Proof.** By Theorem 1, it is enough to consider the case when $G = G(h)$ is a linear benzenoid chain with exactly $h$ hexagons. Define $S(h) = T(G(h), x, y)$. Consider the following five graphs:

- The Graph $G_1(h)$ constructed from G by replacing the end hexagon of G by a triangle, Figure 3(ii);
- The Graph $G_2(h)$ constructed from G by replacing the end hexagon of G by a quadrangle, Figure 3(iii);
- The Graph $G_3(h)$ constructed from G by replacing the end hexagon of G by a pentagon, Figure 3(iv);
- The Graph $G_4(h)$ constructed from G by replacing the end hexagon of G by an edge, Figure 3(v);
- The Graph $G_5(h)$ constructed from $G_1(h)$ by adding a loop to the middle vertex of the pentagon, Figure 3(vi).

To compute the Tutte polynomial of $G$, we proceed by induction on $h$ and obtain a recurrence relation for $S(h)$. We first notice that $S(1) = x^5 + x^4 + x^3 + x^2 + x + y$. Define $S_i(h) = T(G_i(h-1), x, y)$, $1 \le i \le 5$. By deleting an edge from the end hexagon of $G$ with vertices of degree 2 and applying Theorem 1, we can see that

$$\begin{aligned} S(h) &= x^4S(h-1) + S_1(h-1) = x^4S(h-1) + x^3S(h-1) + S_2(h-1) \\ &= x^4S(h-1) + x^3S(h-1) + x^2S(h-1) + S_3(h-1) \\ &= x^4S(h-1) + x^3S(h-1) + x^2S(h-1) + xS(h-1) + S_4(h-1) \\ &= x^4S(h-1) + x^3S(h-1) + x^2S(h-1) + xS(h-1) + S(h-1) + S_5(h-2) \\ &= (x^4 + x^3 + x^2 + x + 1)\, S(h-1) + S_5(h-2). \end{aligned}$$

Therefore

$$S(h) = (x^4+ x^3+ x^2+ x+ 1)\, S(h-1) + S_5(h-2). \tag{1}$$

We now calculate $S_5(h-2)$. To do this, we notice that $S_5(h-2)$ has a loop. Thus

$$S_5(h-2) = yS_1(h-2). \qquad (2)$$

To compute $S_1(h-2)$ we put $h-1$ in $S(h) = x^4S(h-1) + S_1(h-1)$. Thus $S(h-1) = x^4S(h-2) + S_1(h-2)$. Therefore $S_1(h-2) = S(h-1) - x^4S(h-2)$. Apply Eqs. (1) and (2), we have:

$$S(h) = (x^4+ x^3+ x^2+ x+ 1)\, S(h-1) + yS_1(h-2). \qquad (3)$$

Hence,

$$\begin{aligned} S(h) &= (x^4+ x^3+ x^2+ x+ 1)\, S(h-1) + y(S(h-1) - x^4S(h-2)) \\ &= (x^4+ x^3+ x^2+ x+ 1+ y)\, S(h-1) - x^4y\, S(h-2). \end{aligned}$$

This implies that $T(G(h),x,y) = \left(y + \dfrac{x^5-1}{x-1}\right)T(G(h-1),x,y) - x^4yT(G(h-2),x,y)$. There are several methods in discrete mathematics to solve such a recurrence equation. By applying one of these methods, we have

$$T(G,x,y) = \left(\frac{x(J+\sqrt{\Delta}) + 2(1-x)y}{2\sqrt{\Delta}}\right)\left(\frac{J+\sqrt{\Delta}}{2}\right)^n + \left(\frac{x(-J+\sqrt{\Delta}) - 2(1-x)y)}{2\sqrt{\Delta}}\right)\left(\frac{J-\sqrt{\Delta}}{2}\right)^n,$$

where

$$J = x^4 + x^3 + x^2 + x + 1 + y,$$

$$\Delta = (x^4 + x^3 + x^2 + x + 1)^2 + y^2 + 2y(x^4 + x^3 + x^2 + x + 1) - 4x^4y,$$

which completes our proof. □

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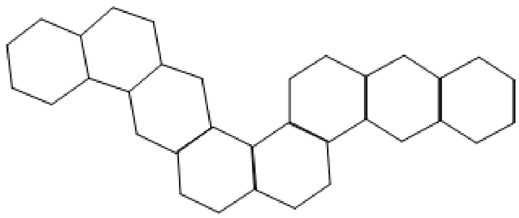
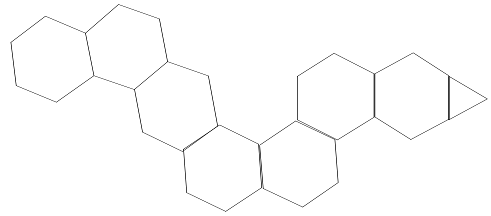
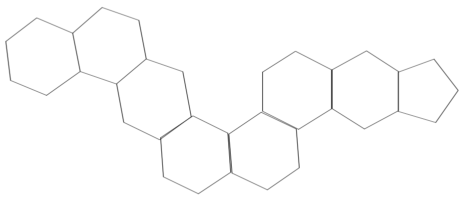
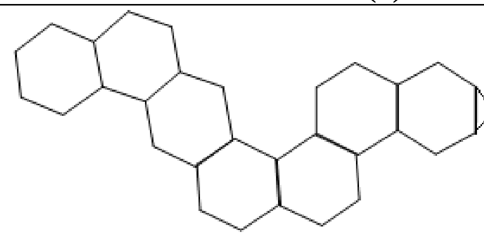
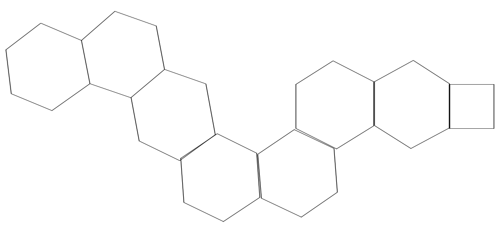
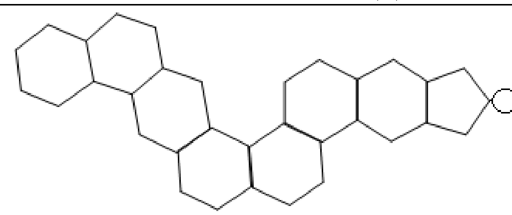
|  |  |
| i) The Graph G(h). | iv) The Graph of $G_3(h-1)$ Constructed From G(h). |
|  |  |
| ii) The Graph $G_1(h-1)$ Constructed From G(h). | v) The Graph $G_4(h-1)$ Constructed From G(h). |
|  |  |
| iii) The Graph $G_2(h-1)$ Constructed From G(h). | vi) The Graph $G_5(h-2)$ Constructed From G(h). |

**Figure 3.** A Graph G(h) and Five Types of Graphs Constructed from G(h).

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