Tutte polynomial of the Stoddart's poly(Ammonium) dendrimer

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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. In this paper a simple method is presented by which it is possible to calculate the Tutte polynomial of dendrimer nanostars.

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1. Introduction

Dendrimers are highly branched macromolecules. In a divergent synthesis of a dendrimer, one starts from the core and growths out to the periphery. In each repeated step, a number of monomers are added to the core, in a radial manner, in resulting quasi concentric shells, called generations. In a convergent synthesis, the periphery is first built up and next the branches are connected to the core. These rigorously tailored structures reach rather soon, between the thirds to tenth generation, depending on the number of connections of degree less than three between the branching points a spherical shape, which resembles that of a globular protein, after that the growth process stops. The stepwise growth of a dendrimer follows a mathematical progression. The size of dendrimers is in the nanometer scale. The endgroups can be functionalized, thus modifying their physico-chemical or biological properties [1]. The graph theoretical study of these macromolecules is the aim of this article [2–11].

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 [12–14]. 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 is defined by the recurrence relation $T_G = T_{G-e} + T_{G/e}$ 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. Especially, $T_G = 1$ if *G* contains no edges. In this paper, we compute tute polynomial of Ns[n] Figs. 1 – 3.

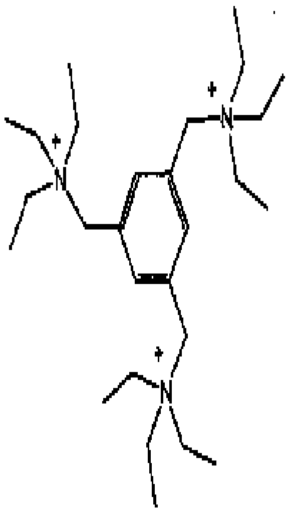

Fig. 1. The Molecular Graph of Ns[0].

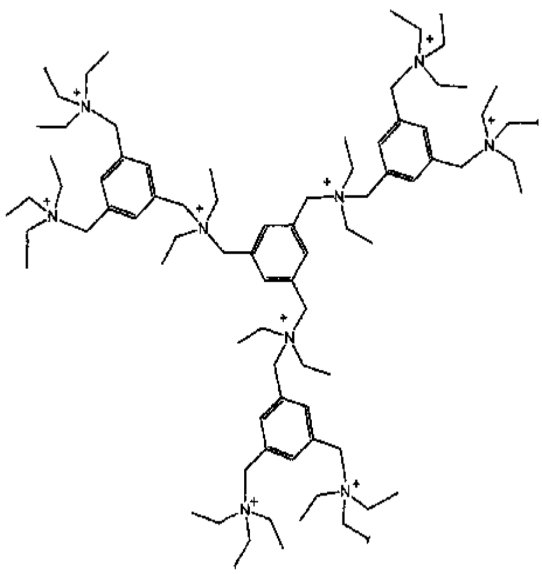

Fig. 2. The Molecular Graph of Ns[1].

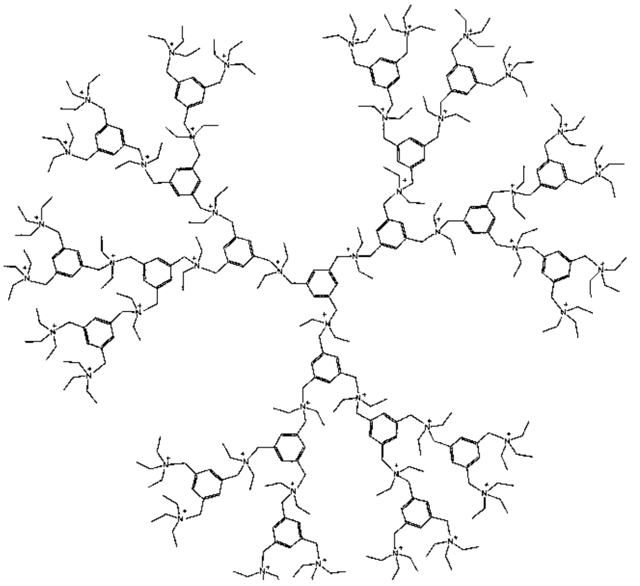

Fig. 3. The 2-Dimentional Lattice of Ns[3].

The main result of this paper is the following theorem:

Theorem. $T(D[n],\ x,\ y) = x^{24\left(2^{n+1}-1\right)}\left(\dfrac{x^6-x}{x-1}+y\right)^{3\times 2^n-2}$.

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 Stoddart's poly (ammonium) dendrimer, D[n], is computed. We first introduce some important notions. 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 α is reflexive. Moreover, we can easily prove that α is symmetric and transitive. So α is an equivalence relation on $V(G)$. The equivalence classes of α is called the *connected components* of G. One can define the Tutte polynomial as $T(G,x,y) = \Sigma_{A\subseteq E}(x-1)^{c(A)-c(E)}(y-1)^{c(A)+|A|-|V|}$. Here, c(A) denotes the number of connected components of the graph (V,A).

To compute the Tutte polynomial of D[n], we proceed inductively. To do this, we first compute T(D[0],x,y).

Lemma 1. $T(D[0],\ x,\ y) = x^{24}\left(\dfrac{x^6-x}{x-1}+y\right)$.

Theorem. $T(D[n],\ x,\ y) = x^{24\left(2^{n+1}-1\right)}\left(\dfrac{x^6-x}{x-1}+y\right)^{3\times 2^n-2}$.

Proof. Suppose e[n], v[n], b[n] and h[n] denote the number of edges, vertices, bridges and hexagons of D[n], respectively. It is easy to see that $b[n] = 3 \times 2^n + b[n-1]$ and $h[n] = 3 \times 2^{n-1} + h[n-1]$. On the other hand, $T(C_6,x,y) = T(P_6,x,y) + T(C_5,x,y) = T(P_6,x,y) + T(P_5,x,y) + T(C_4,x,y) = T(P_6,x,y) + T(P_5,x,y) + T(P_4,x,y) + T(C_3,x,y) = \left(\dfrac{x^6-x}{x-1}+y\right)$. By an inductive argument and a tedious calculation, one can see that

$$T(D[n],\ x,\ y) = x^{24\left(2^n\right)}\left(\frac{x^6-x}{x-1}+y\right)^{3\times 2^{n-1}} T(D[n-1],\ x,\ y)$$

and so $\dfrac{T(D[n],\ x,\ y)}{T(D[n-1],\ x,\ y)} = x^{24\left(2^n\right)}\left(\dfrac{x^6-x}{x-1}+y\right)^{3\times 2^{n-1}}$. Thus

$$\prod_{n=1}^{m}\frac{T(D[n],\ x,\ y)}{T(D[n-1],\ x,\ y)} = \prod_{n=1}^{m} x^{24\left(2^n\right)}\left(\frac{x^6-x}{x-1}+y\right)^{3\times 2^{n-1}}.$$

This implies that

$\dfrac{T(D[n],\ x,\ y)}{T(D[0],\ x,\ y)} = x^{48\left(2^n-1\right)}\left(\dfrac{x^6-x}{x-1}+y\right)^{3\times(2^n-1)}$. Therefore

$$T(D[n],\ x,\ y) = x^{48\left(2^n-1\right)}\left(\frac{x^6-x}{x-1}+y\right)^{3\times(2^n-1)} T(D[0],\ x,\ y).$$

We now apply Lemma 1 to deduce that:

$$T(D[n],\ x,\ y) = x^{48\left(2^n-1\right)}\left(\frac{x^6-x}{x-1}+y\right)^{3\times(2^n-1)} x^{24}\left(\frac{x^6-x}{x-1}+y\right)$$

$$= x^{24\left(2^{n+1}-1\right)}\left(\frac{x^6-x}{x-1}+y\right)^{3\times 2^n-2}.$$

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