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TUTTE POLYNOMIAL OF AN INFINITE CLASS OF NANOSTAR DENDRIMERS

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ABSTRACT. Tutte polynomial T(G,x,y), is a precise topological description of an undirected graph G with two variables, which gives some information about the connectivity of the graph. Dendrimers are hyper-branched nano-structures with rigorously tailored architecture. In this paper, the formula for Tutte polynomial of an infinite nanostar dendrimer is derived.

Keywords: *Dendrimer, Tutte polynomial.*

INTRODUCTION

Dendrimers are hyper-branched macromolecules showing a rigorous, aesthetically appealing, architecture. They are synthesized, in a controlled manner, basically by two strategies: the *divergent* and *convergent* approaches. In the *divergent methods*, dendrimers are built up starting from a core out to the periphery. In each repeated step, a number of monomer units react with the end groups of the already existing periphery to add a new shell or generation. By each successive generation, the number of local coupling reactions increases. In the *convergent approach*, dendrimers are built from the periphery towards the central core. These rigorously tailored structures show, often at the fifth generation, a spherical shape, which resembles that of a globular protein. The size of dendrimers reaches the nanometer scale. The end groups can be functionalized, thus modifying their physico-chemical or biological properties [1]. Dendrimers have gained a wide range of applications in supramolecular chemistry, particularly in host-guest reactions and self-assembly processes [2-4]; their molecular graphs have been studied by the Mathematical-Chemistry tools [5-7].

Tutte polynomial T(G,*x*,*y*), is a precise topological description of an undirected graph G with two variables, which gives some information about the connectivity of the graph [8]. In order to define Tutte polynomial we need some notations.

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Suppose *G* is an undirected graph with the vertex set V(G) and the edge set E(G). Next, $e \in E(G)$ is neither a loop nor a bridge, then G-*e* is a graph in which the edge *e*=*uv* has been removed. The *edge contraction* G*e* is obtained by linking the endpoints of edge *e*=*uv* together and making that edge as one vertex, (Figure 3). Then the Tutte polynomial of G is defined by the recurrence relation T(G) = T(G-*e*) + T(G*e*). If *G* contains just *i* bridges and *j* loops, T(G,*x*,*y*) = $x^i y^j$. Also, T_G = 1 when *G* has no edges. By the above mathematical notations, we have:

$$\mathrm{T}(G,x,y) = \begin{cases} 1 & \text{if } E(G) = \varnothing \\ x\mathrm{T}(G\text{-}uv,x,y) & \text{if } uv \text{ is a bridge edge} \\ y\mathrm{T}(G\text{-}e,x,y) & \text{if } e \text{ is a loop,} \\ \mathrm{T}(G\text{-}uv,x,y)+\mathrm{T}(G\backslash uv,x,y) & \text{otherwise} \end{cases}.$$

In this paper, we derive the formula for computing the Tutte polynomial of the Nanostar Dendrimer Ns[n], Figure 1.

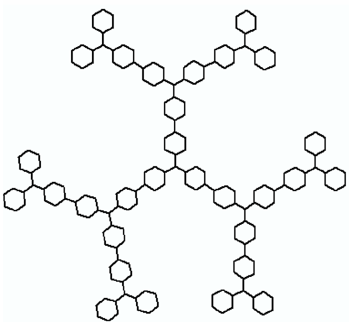

Figure 1. Nanostar dendrimer Ns[2].

MAIN RESULTS

Suppose *G* is an undirected graph with the vertex set V(G) and the edge set E(G). The vertices *v* and *u* of V(G), are in relation α (*v*α*u*), if there is a path in *G* connecting u and v. Each vertex is a path of length zero; so α is a reflexive relation. Moreover, we can easily prove that α is both symmetric and transitive. Thus α is an equivalence relation on *V*(*G*), and its equivalence classes are called the *connected components* of *G*. Then the Tutte polynomial is defined as,

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

where, c(A) denotes the number of connected components of the graph of the vertex set V and the edge set A.

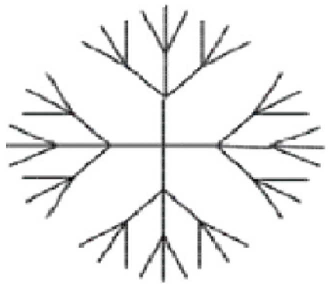

Figure 2. Denderimer D[2].

For example, let G be a tree with n vertices, then T(G, x, y) = x^{n-1}, because all the edges in a tree are bridges. The dendrimer D[n] in Figure 2 is a tree with $2\times3^{n+1}$-1 vertices, thus $T(D[n],x,y)=x^{2\times3^{n+1}-2}$.

The Figure 1 has been constructed by joining six Ns[0] units to the hexagons in the outer layers, as detailed in Figures 3 and 4.

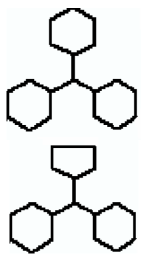

Figure 3. Ns[0] and Ns[0]-H_1+C_5.

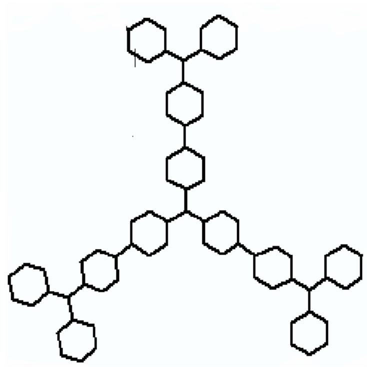

Figure 4. Ns[1].

Lemma 1. Let H be a hexagon. Then $\mathrm{T(D[H],x,y)}=\left(\frac{x^6-x}{x-1}+y\right)$.

Proof. By using the formula of Tutte polynomial, we have:

$$\begin{aligned}\mathrm{T(D[H],\ x,\ y)} &= \mathrm{x^5} + \mathrm{T(D[C_5],\ x,\ y)}\\ &= \mathrm{x^5} + x^4 + \mathrm{T(D[C_4],\ x,\ y)}\\ &= \mathrm{x^5} + x^4 + x^3 + \mathrm{T(D[C_3],\ x,\ y)}\\ &= \frac{x^6-x}{x-1}+y.\end{aligned}$$

To compute the Tutte polynomial of Ns[n], we proceed inductively but at first, we compute T(Ns[0], x, y) in the following

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

Proof. Suppose H_1, H_2 and H_3 are hexagons in Ns[0]; then

$$\begin{aligned}
T(Ns[0],\ x,\ y) &= x^5\, T(Ns[0] - H_1,\ x,\ y) + T(Ns[0] - H_1 + C_5,\ x,\ y) \\
&= x^5\, T(Ns[0] - H_1,\ x,\ y) + x^4\, T(Ns[0] - H_1,\ x,\ y) + \\
&\qquad T(Ns[0] - H_1 + C_4,\ x,\ y) \\
&= x^5\, T(Ns[0] - H_1,\ x,\ y) + x^4\, T(Ns[0] - H_1,\ x,\ y) + \\
&\qquad x^3\, T(Ns[0] - H_1,\ x,\ y) + T(Ns[0] - H_1 + C_3,\ x,\ y) \\
&= \left(\frac{x^6-x}{x-1}+y\right) T(Ns[0]-H_1,x,y),
\end{aligned}$$

where Ns[0]-H_1 + C_i is constructed from Ns[0] by removing H_1 and replacing C_i . As we did in the above,

$$T(Ns[0], x, y)= \left(\frac{x^6-x}{x-1}+y\right)^2 T(Ns[0]-H_1-H_2,x,y).$$

Thus, T(Ns[0], x, y) = $\left(\frac{x^6-x}{x-1}+y\right)^3 T(Ns[0]-H_1-H_2-H_3,x,y)$. This implies that

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

Lemma 3. T(Ns[1], x, y) = $x^{15}\left(\frac{x^6-x}{x-1}+y\right)^{12}$.

Proof. By a similar proof as Lemma 2, we can see that

$$T(Ns[1], x, y) = \left(\frac{x^6-x}{x-1}+y\right)^9 x^{12} T(Ns[0],x,y).$$

Thus, T(Ns[1], x, y) = $x^{15}\left(\frac{x^6-x}{x-1}+y\right)^{12}$.

Theorem 4. T(Ns[n], x, y) = $x^{2\times 4^{n+1}+7}\left(\frac{x^6-x}{x-1}+y\right)^{9\times 2^n-6}$.

Proof. Suppose b[n] and h[n] denote the number of bridges and hexagons of Ns[n], respectively. It is easy to see that b[n] = $2 \times 4^{n+1} + 7$ and h[n] = $9\times 2^n - 6$. Thus b[n] = b[n-1] + 6×4^n bridges and h[n] = h[n-1]+$9\times 2^{n-1}$ hexagons. Now, by using the definition of Tutte polynomial for bridges and hexagons of Ns[n] - Ns[n-1], and lemma 2, we have

$$\mathrm{T(Ns[n],\ x,\ y)} = \mathrm{x}^{6\times 4^{n}}\left(\frac{x^6-x}{x-1}+y\right)^{9\times 2^{n-1}} T(Ns\,[n-1],\, x, y).$$

For solving this recursive sequence, we write

$$\prod_{m=2}^{n}\frac{\mathrm{T(Ns[m],\ x,\ y)}}{T(Ns\,[m-1],\, x, y)} = \prod_{\mathrm{m}=2}^{\mathrm{n}}\mathrm{x}^{6\times 4^{m}}\left(\frac{x^6-x}{x-1}+y\right)^{9\times 2^{m-1}}.$$

This implies that

$$\mathrm{T(Ns[n],\ x,\ y)} = \mathrm{x}^{2\times 4^{n+1}-8}\left(\frac{x^6-x}{x-1}+y\right)^{9\times 2^{n}-18} T(Ns\,[1],\, x, y).$$

Therefore by Lemma 3,

$$\mathrm{T(Ns[n],\ x,\ y)} = \mathrm{x}^{2\times 4^{n+1}+7}\left(\frac{x^6-x}{x-1}+y\right)^{9\times 2^{n}-6}.$$

This completes the proof.

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