Computing Chemical Properties of Molecules by Graphs and Rank Polynomials

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ABSTRACT

The topological index of a graph G is a numeric quantity related to G which is invariant under automorphisms of G. The Tutte polynomial of G is a polynomial in two variables defined for every undirected graph contains information about connectivity of the graph. The Padmakar-Ivan, vertex Padmakar-Ivan polynomials of a graph G are polynomials in one variable defined for every simple connected graphs that are undirected. In this paper, we compute these polynomials of two infinite classes of dendrimer nanostars.

Keywords: Dendrimers, Tutte polynomial, PI-polynomial.

1. INTRODUCTION

Dendrimers are repeatedly branched, roughly spherical large molecules. 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 the 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

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dendrimers is in the nanometer scale. The end groups 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, see [2,3] for details.

Let $G = (V, E)$ be a simple graph with the vertex and edge sets V and E, respectively. The graph theory has successfully provided chemists with a variety of very useful tools, namely, counting polynomial. The Tutte polynomial is one of such polynomials. This polynomial has two variables which contains information about how the graph is connected [4–6] 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. The Rutte 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 $R_G(x, y) = (x + 1)^i (y + 1)^j$ if G contains i bridges and j loops and no other edges [7]. Especially, $R_G = 1$ if G contains no edges. In this paper, we compute the Tutte polynomial of dendrimer D[n] and Ns[n], see Figures [1-4].

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

2. MAIN RESULTS AND DISCUSSION

A topological index of a graph is a number invariant under its automorphisms. The simplest topological indices are the number of vertices and edges of the graph. The Wiener index W is one of the oldest topological indices introduced by Harold Wiener. We know that the distance between the edge $f = xy$ and the vertex u in the graph G is denoted by $d_G(f, u)$ and is define by $d_G(f, u) = \min\{d_G(x, u), d_G(y, u)\}$. Let $e = uv$ be an edge of the graph G, then can define the sets $M(e, u, G) = \{f \in E(G) | d_G(f, u) < d_G(f, v)\}$; $M(e, v, G) = \{f \in E(G) | d_G(f, v) < d_G(f, u)\}$, $m_u(e) = m_u(e, G) = |M(e, u, G)|$ and $m_v(e) = m_v(e, G) = |M(e, v, G)|$. Define the sets $(e, u, G) = \{x \in V(G) | d_G(x, u) < d_G(x, v)\}$; $N(e, v, G) = \{x \in V(G) | d_G(x, v) < d_G(x, u)\}$, $n_u(e) = n_u(e, G) = |N(e, u, G)|$ and $n_v(e) = n_v(e, G) = |N(e, v, G)|$ [8,9].

In this section the Tutte, PI and PI_v polynomials of the graph of the molecular graphs of D[n] and T–benzyl–terminated amide–based dendrimers, Ns[n], are computed. To compute, we notice that this graph is a tree and so every edge is a bridge. Thus, $|V(D[n])| = 3^{n+1} - 1$ and $|E(D[n])| = 3^{n+1} - 2$.

Theorem 1. $PI(D[n], x) = (3^{n+1} - 2)x^{(3^{n+1}-3)}$ and $PI_v(D[n], x) = (3^{n+1} - 2)x^{(3^{n+1}-1)}$.

Proof. For every edge $e = uv$, we have:

$$m_u(e) + m_v(e) = |E(D[n])| - 1 = 3^{n+1} - 3 \text{ and } n_u(e) + n_v(e) = 3^{n+1} - 1.$$

Therefore,

$$PI(D[n], x) = \sum_{e=uv} x^{[\,m_u(e)+m_v(e)\,]} = \sum_{e=uv} x^{(3^{n+1}-3)} = (3^{n+1} - 2)x^{(3^{n+1}-3)} \text{ and}$$

$$PI_v(D[n], x) = \sum_{e=uv} x^{[\,n_u(e)+n_v(e)\,]} = \sum_{e=uv} x^{(3^{n+1}-1)} = (3^{n+1} - 2)x^{(3^{n+1}-1)}$$

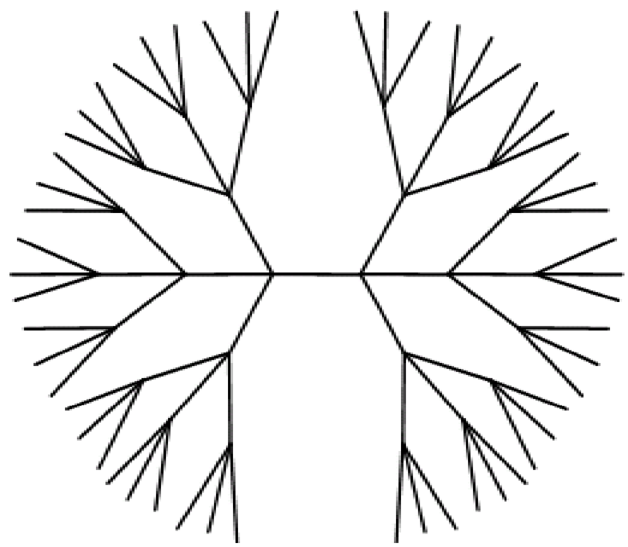

Figure 1. Denderimer D[3].

Now we introduce some important notions. Suppose that 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 Rank polynomial of D[n], we proceed inductively. To do this, we first compute the value of R(D[n], x, y).

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

Proof. Dendrimer D[n] has 3^{n+1}-2 bridge edges. Thus by definition of Tutte polynomial,

$$R(D[n], x, y) = (x+1)^{\left(3^{n+1}-2\right)}.$$

Now for constructing Figure 4, we put Figure 2 on Figure 3 by joining N to A.

Lemma 3. Suppose that H be a hexagon. Then

$$R(D[H],x,y) = \left(\frac{(x+1)^6-x-1}{x}+y+1\right).$$

Proof. By definition of Rank polynomial, we have

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

Lemma 4. If G be a tree, then R(G, x, y) = $(x+1)^{n-1}$.

To compute the above polynomials of Ns[n], we assume that e[n], v[n], b[n] and h[n] denote the number of edges, vertices, bridges and hexagons of Ns[n], respectively. We can see

e[n] = b[n] + 6h[n] = $13 \times 2^{n+1} - 9$,
v[n] = b[n] + 1 +5h[n] = $12 \times 2^{n+1} - 8$,
b[n] = $7 \times 2^{n+1}$ - 9 and
h[n] = 2^{n+1}.

Lemma 5. Let $e = uv$ be an edge of Ns[n], then
a) If e is a bridge, then $m_u(e)+m_v(e)$ = e[n]−1.
b) If e is an edge of a hexagon, then $m_u(e)+m_v(e)$ = e[n] −2.
c) $n_u(e)+n_v(e)$ = v[n].

Proof. Notice that if e is a bridge, then e is the only edge being equidistance to its end vertices and if e is an edge of a hexagon, then e has only two equidistance edges to u and v. Also in both cases, every edge of Ns[n] is belonging to $N(e,u,G) \cup N(e,v,G)$ and our proof is complete.

Theorem 6. $PI(Ns[n],x) = (7 \times 2^{n+1} - 9)x^{(13\times 2^{n+1}-10)} + 6 \times 2^{n+1}x^{(13\times 2^{n+1}-11)}$ and $PI_v(Ns[n],x) = (13 \times 2^{n+!} - 9)x^{12\times 2^{n+1}} - 8$.

Proof. Let B be the set of all bridge and H be the set of all edges of the hexagons of Ns[n]. Then we have:

$$PI(Ns[n],x) = \sum_{e=uv} x^{[m_u(e)+m_v(e)]} = \sum_{e=uv\in B} x^{[m_u(e)+m_v(e)]} + \sum_{e=uv\in H} x^{[m_u(e)+m_v(e)]}$$

$$= \sum_{e=uv\in B} x^{e[n]-1} + \sum_{e=uv\in H} x^{e[n]-2} = b[n]x^{e[n]-1} + 6h[n]x^{e[n]-2}$$

$$= (7\times 2^{n+1}-9)x^{(13\times 2^{n+1}-10)} + 6\times 2^{n+1}x^{(13\times 2^{n+1}-11)}$$

$$PI_v(Ns[n],x) = \sum_{e=uv} x^{[n_u(e)+n_v(e)]} = \sum_{e=uv} x^{v[n]} = (13\times 2^{n+1}-9)x^{(12\times 2^{n+1}-8)}.$$

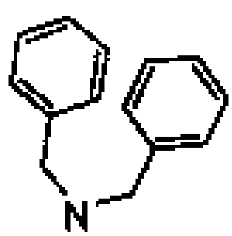

Figure 2. A Piece of Ns[n].

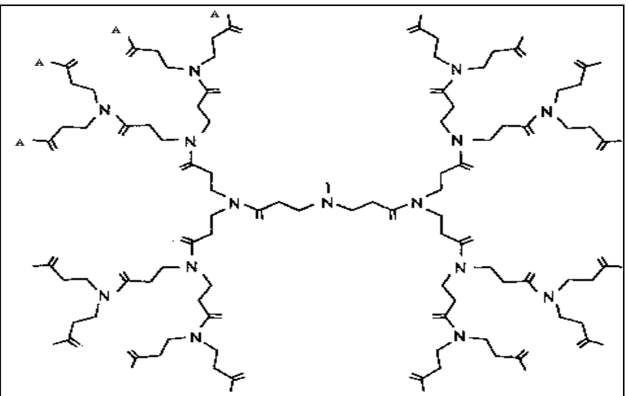

Figure 3. A Piece of Ns[n] Denoted by G.

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

Proof. By the definition of Rank polynomial for edges on hexagon and Lemma3, we can see

$$R(Ns[n],x,y) = \left(\frac{(x+1)^6-x-1}{x}+y+1\right)^{2^{n+1}} R(G,x,y),$$

where G is the subgraph of Ns[n] made of all bridges. But G is a tree with $7\times 2^{n+1}-9$ edges. Thus by Lemma 4,

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

This completes the proof.

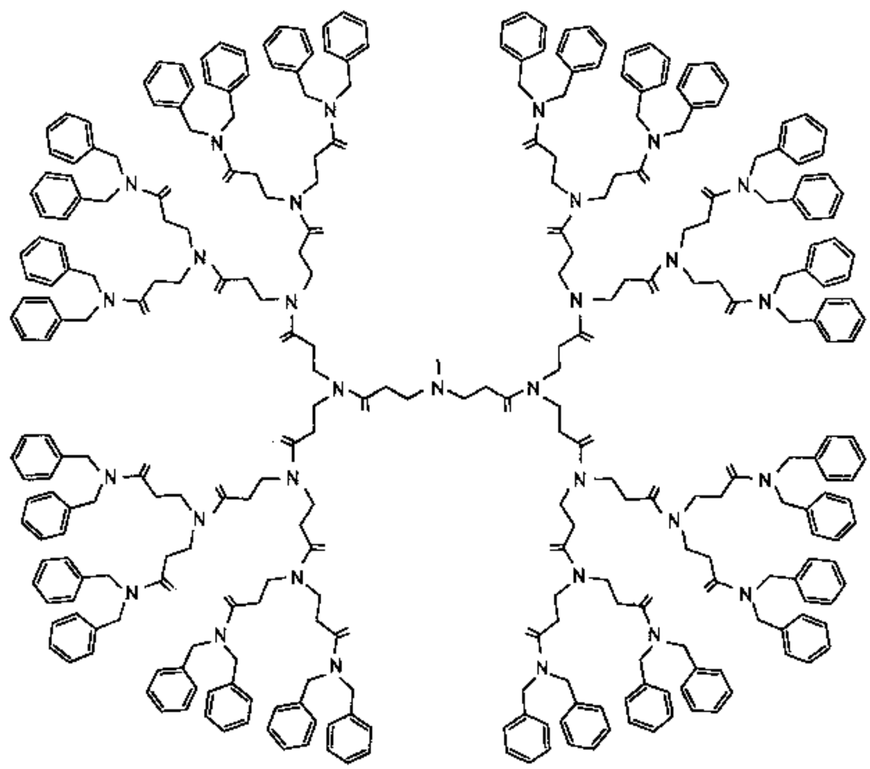

Figure 4. T-benzyl-terminated amide-based dendrimers, Ns[4].

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