Computing chemical properties of molecules by graphs

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Suppose that G is a 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. Also the Tutte polynomial of G is a polynomial in two variables defined for every undirected graph contains information about how the graph is connected. In this paper, we compute these polynomials of two infinite classes of dendrimer nanostars.

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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 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 [2–10].

Let $G = (V,E)$ be a simple graph where V and E are the vertex and edge sets of the graph G, respectively. The graph theory has successfully provided chemists with a variety of very useful tools, namely, the topological indices. 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
$m_v(e) = m_v(e,G) = |M(e,v,G)|$.

Also can define the sets

$N(e,u,G) = \{x \in V(G) | d_G(x,u) < d_G(x,v)\}$;
$N(e,v,G) = \{x \in V(G) | d_G(x,v) < d_G(x,u)\}$,
$n_u(e) = n_u(e,G) = |N(e,u,G)|$ and
$n_v(e) = n_v(e,G) = |N(e,v,G)|$.

It is obvious that an end-vertex of any edge is closer to itself than to the other end-vertex of that edge. Hence the sum $n_u(e)+n_v(e)$ is always positive.

The Padmakar-Ivan and the vertex Padmakar-Ivan polynomials of a graph G are polynomials in one variable that is defined as follows, respectively.

$$PI(G,x) = \sum_{e=uv} x^{[m_u(e)+m_v(e)]} \quad ;$$

$$PI_v(G,x) = \sum_{e=uv} x^{[n_u(e)+n_v(e)]} .$$

It is clear that the derivation of these polynomials for $x = 1$ are $PI(G)$ and $PI_v(G)$, respectively. 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 [11–14]. 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 Padmakar-Ivan, the vertex Padmakar-Ivan and Tute polynomials of D[n] and Ns[n] Figs. 1–4.

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

2. Main results

In this section the Padmakar-Ivan, vertex Padmakar-Ivan and Tutte polynomials of the graph of D[n] and T-benzyl-terminated amide-based dendrimers, Ns[n], are computed.

To compute the Padmakar-Ivan and vertex Padmakar-Ivan polynomials of D[n], note that this graph is a tree and every edge is a bridge. So $|V(D[n])| = 3^{n+1} - 1$ and $|E(D[n])| = 3^{n+1} - 2$.

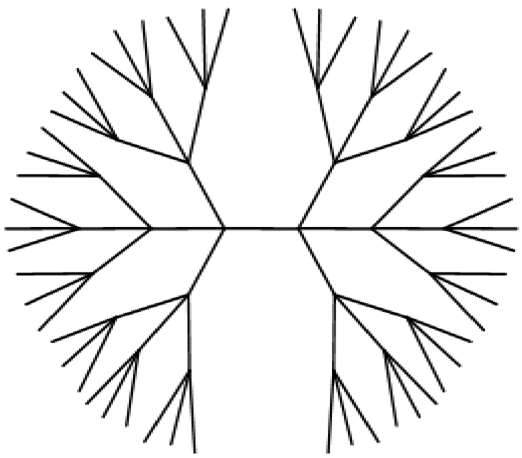

Fig. 1. Denderimer D[3].

Theorem1.

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

Proof. For every edge $e = uv$,

$$m_u(e) + m_v(e) = |E(D[n])| - 1 = 3^{n+1} - 3$$

and $n_u(e) + n_v(e) = |V(D[n])| = 3^{n+1} - 1.$

Therefore

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

and

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

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

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

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

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

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

Lemma3. Suppose that H be a hexagon. Then $T(D[H], x, y) = \left(\frac{x^6 - x}{x-1} + y\right)$.

Proof. By definition of Tutte polynomial, we have

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

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

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. Can see

$$e[n] = b[n] + 6h[n] = 13 \times 2^{n+1} - 9,$$

$$v[n] = b[n] + 1 + 5h[n] = 12 \times 2^{n+1} - 8,$$

$$b[n] = 7 \times 2^{n+1} - 9 \text{ and}$$

$$h[n] = 2^{n+1}.$$

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. Note 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 edges of Ns[n] is belong 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 hexagons of Ns[n]. Then

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

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

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

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

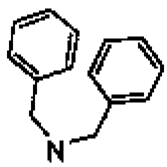

Fig. 2. A piece of Ns[n].

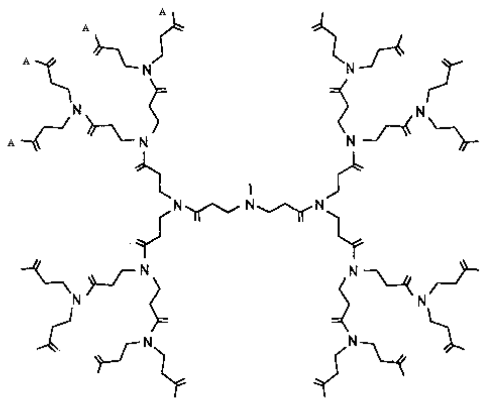

Fig. 3. A piece of Ns[n] denoted by G.

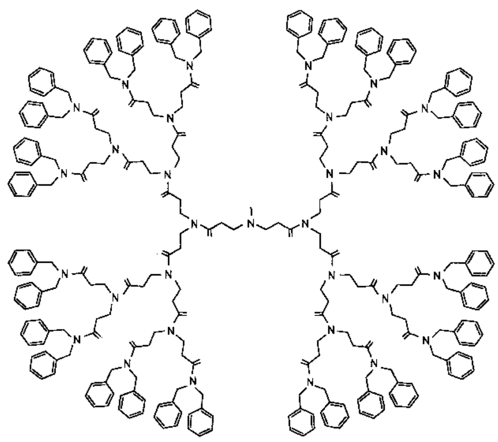

Fig. 4. T-benzyl-terminated amide-based dendrimers, Ns[4].

Theorem7.

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

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

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

where G is the subgraph of Ns[n] made of all bridges. But G is a tree with $7\times2^{n+1}$-9 edges. Thus by Lemma 4

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

This completes the proof.

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