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CHROMATIC POLYNOMIALS OF CERTAIN FAMILIES OF DENDRIMER NANOSTARS

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Let G be a simple graph and $\lambda \in \mathbb{N}$. A mapping $f : V(G) \to \{1,2,\ldots,\lambda\}$ is called a λ-colouring of G if $f(u) \neq f(v)$ whenever the vertices u and v are adjacent in G. The number of distinct λ-colourings of G, denoted by $P(G,\lambda)$ is called the chromatic polynomial of G. A dendrimer is an artificially manufactured or synthesized molecule built up from branched units called monomers. In this paper, using the chromatic polynomial of some specific graphs, we compute the chromatic polynomials for certain families of dendrimer nanostars.

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1. Introduction

A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a (possibly empty) set $E(G)$ of unordered pairs of distinct vertices of G called edges. In chemical graphs, the vertices of the graph correspond to the atoms of the molecule, and the edges represent the chemical bonds.

Let $\chi(G,\lambda)$ denotes the number of proper vertex colourings of G with at most λ colours. G. Birkhoff [4], observed in 1912 that $\chi(G,\lambda)$ is, for a fixed graph G, a polynomial in λ, which is now called the chromatic polynomial of G. More precisely, let G be a simple graph and $\lambda \in \mathbb{N}$. A mapping $f : V(G) \to \{1,2,\ldots,\lambda\}$ is called a λ-*colouring* of G if $f(u) \neq f(v)$ whenever the vertices u and v are adjacent in G. The number of distinct λ-colourings of G, denoted by $P(G,\lambda)$ is called the *chromatic polynomial* of G. The book by F.M. Dong, K.M. Koh and K.L. Teo [5] gives an excellent and extensive survey of this polynomial.

A *topological index* is a real number related to a graph. It must be a structural invariant, i.e., it is fixed by any automorphism of the graph. There are several topological indices have been defined and many of them have found applications as means to model chemical, pharmaceutical and other properties of molecules. The Wiener index W and diameter are two examples of topological indices of graphs (or chemical model). For a detailed treatment of these indices, the reader is referred to 9,10.

Dendrimers are hyper-branched macromolecules, with a rigorously tailored architecture. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. Dendrimers have gained a wide range of applications in supra-molecular chemistry, particularly in host guest reactions and self-assembly processes. Their applications in chemistry, biology and nano-science are unlimited. Recently, some people investigated the mathematical properties of

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these nanostructures in [3,6,10,11,12]. Also Alikhani and Iranmanesh [1,2] investigated the chromatic polynomials of some nanotubes and dendrimers. In this paper we would like to investigate some further results on chromatic polynomials of certain families of dendrimer nanostars.

In Section 2, we state two graphs with specific structures with their chromatic polynomials. Using the results in Section 2, we study the chromatic polynomials of certain families of dendrimer nanostars in Section 3.

2. Chromatic polynomials of certain graphs

In this section we consider some specific graphs and state their chromatic polynomials.

Let P_{m+1} be a path with vertices labeled by $y_0, y_1, ..., y_m$ for $m \geq 0$ and let G be any graph. Denote by $G_{v_0}(m)$ (simply $G(m)$) a graph obtained from G by identifying the vertex v_0 of G with an end vertex y_0 of P_{m+1} (see Figure 1). For example, if G is a path P_2, then $G(m) = P_2(m)$ is the path P_{m+2}.

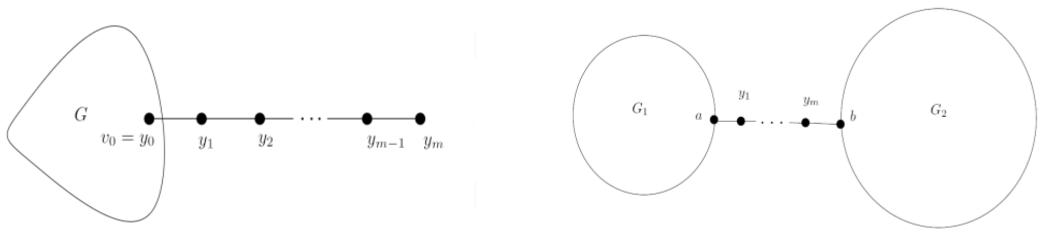

Fig. 1. Graphs $G(m)$ and $G_1(m)G_2$, respectively.

Theorem 1 (Alikhani and Iranmanesh [2]). *Let $m \in \mathbb{N}$. Then, the chromatic polynomial of $G(m)$ is*

$$P(G(m), \lambda) = (\lambda - 1)^m P(G, \lambda).$$

Let G_1 and G_2 be graphs, each containing a complete subgraph K_p with p vertices. If G is the graph obtained from G_1 and G_2 by identifying the two subgraphs K_p, then G is called a K_p-gluing of G_1 and G_2. Note that a K_1-gluing and a K_2-gluing are also called a vertex-gluing and an edge-gluing, respectively.

The following theorem gives the formula for computing the chromatic polynomial of graphs $G_1(m)G_2$ as shown in Figure 1.

Theorem 2 (Alikhani and Iranmnesh [2]). *Let $m \in \mathbb{N}$. The chromatic polynomial of $G_1(m)G_2$ is*

$$P(G_1(m)G_2, \lambda) = \frac{(\lambda - 1)^{m+1}}{\lambda} P(G_1, \lambda) P(G_2, \lambda).$$

Theorem 2 implies that all forms of $G_1(m)G_2$ have the same chromatic polynomials.

We need the following lemma to obtain our main results.

Lemma 1 (Farrel [7]). Let G be a graph with n vertices and m edges. Then in the chromatic polynomial $P(G, \lambda)$,

(i) deg $(P(G,\lambda)) = n$,

(ii) the coefficient of λ^n is 1,
(iii) the coefficient of λ^{n-1} is – *m*.

3. Chromatic polynomials of some dendrimer nanostars

In this section we shall compute the chromatic polynomials of some dendrimer nanostars. First we compute the chromatic polynomial of the class of dendrimer nanostars known as PAMAM dendrimer with trifunctional core unit by construction of dendrimer generations G_n has grown *n* stages. We denote simply this graph by $PD_1[n]$. Figure 2 shows generations G_3 has grown 3 stages.

Theorem 3. Let $n \in N_0$. The chromatic polynomial of $PD_1[n]$ is

$$P(PD_1[n],\lambda) = \lambda(\lambda-1)^{12\times 2^{n+2}-24}.$$

Proof. By induction on *n*. Since $P(PD_1[0],\lambda) = \lambda(\lambda-1)^{24}$, the result is true for *n* = 0. Now suppose that the result is true for less than *n* and we prove it for *n*.
Since $P(PD_1[n],\lambda) = P(PD_1[n-1]\times \underbrace{T_{17}}_{3\times 2^{n-1}-times},\lambda)$, by Theorem 2, we have

$$P(PD_1[n],\lambda) = P(PD_1[n-1])\left(\frac{P(T_{17},\lambda)}{\lambda}\right)^{3\times 2^{n-1}}.$$

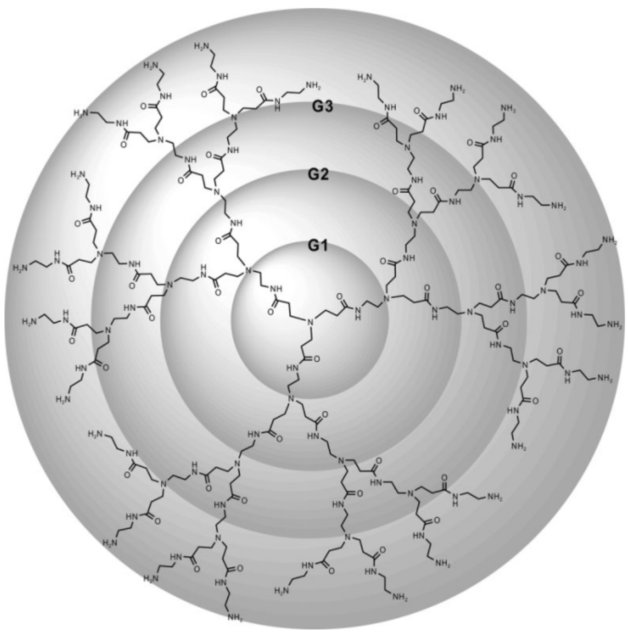

Fig. 2. PAMAM dendrimer of generations G_n has grown 3 stages.

Now by induction hypothesis, we obtain

$$P(PD_1[n],\lambda) \;=\; \lambda(\lambda-1)^{12x2^{n+1}-24}.\left(\frac{P(T_{17},\lambda)}{\lambda}\right)^{3\times 2^{n-1}}$$

$$= \lambda(\lambda-1)^{12\times 2^{n+1}-24} . \left(\frac{\lambda(\lambda-1)^{16}}{\lambda}\right)^{3\times 2^{n-1}}$$
$$= \lambda(\lambda-1)^{12\times 2^{n+1}-24} .\ (\lambda-1)^{16\times 3\times 2^{n-1}}$$
$$= \lambda(\lambda-1)^{12\times 2^{n+2}-24}.$$

Now we have the following corollary by Theorem 3.

Corollary 1. (i) The order of $PD_1[n]$ is $|V(PD_1[n])| = 12\times 2^{n+2} - 23.$

(ii) The size of $PD_1[n]$ is $|E(PD_1[n])| = 12\times 2^{n+2} - 24.$

Proof. (i) Using Lemma 1(i), $\deg(P(G,\lambda)) = |V(G)|$. By Theorem 3, $\deg(P(PD_1[n],\lambda)) = 12\times 2^{n+2} - 23.$ Therefore $|V(PD_1[n])| =$ $12\times 2^{n+2} - 23.$

(ii) Using Lemma 1(iii), the coefficient of $\lambda^{|V(G)|-1}$ is the number of edges of $G.$ By Theorem 3, $|E(PD_1[n])| = 12\times 2^{n+2} - 24.$

Now we shall compute the chromatic polynomials of another type of PAMAM dendrimers different core by construction of dendrimer generations G_n has grown *n* stages. We denote simply this graph by $PD_2[n].$ Figure 3 shows the generations G_3 has grown 3 stages.

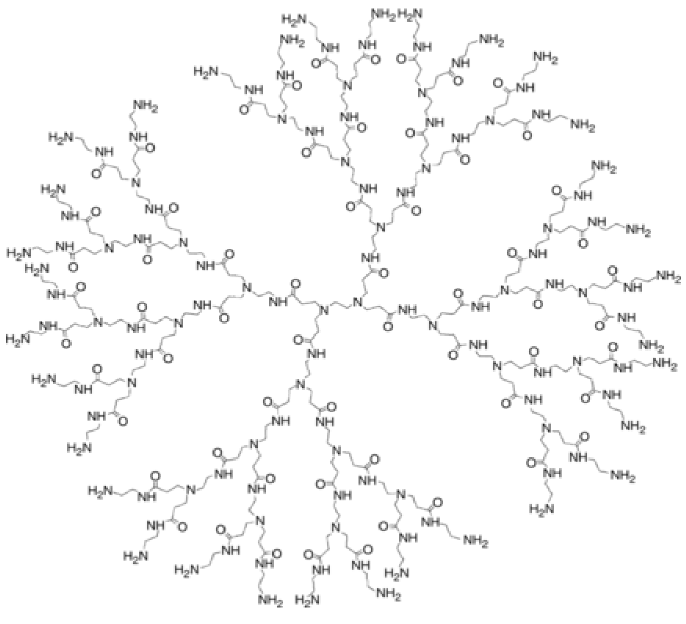

Fig. 3. PAMAM dendrimer of generation G_n has grown 3 stages.

Theorem 4. Let $n \in N_0$. The chromatic polynomial of $PD_2[n]$ is

$$P(PD_2[n],\lambda) = \lambda(\lambda-1)^{16\times 2^{n+2}-29}.$$

Proof. By induction on *n*. Since $P(PD_2[0],\lambda) = \lambda(\lambda-1)^{35}$, the result is true for *n* = 0. Now suppose that the result is true for less than *n* and we prove it for *n*. Since $P(PD_2[n],\lambda) = P(PD_2[n-1]\times \underbrace{T_{17}}_{2^{n+1}-times},\lambda)$, by Theorem 2, we have

$$P(PD_2[n],\lambda) = P(PD_2[n-1])\left(\frac{P(T_{17},\lambda)}{\lambda}\right)^{2^{n+1}}.$$

Now by induction hypothesis, we obtain

$$P(PD_2[n],\lambda) = \lambda(\lambda-1)^{16x2^{n+1}-29}.\left(\frac{P(T_{17},\lambda)}{\lambda}\right)^{2^{n+1}}$$

$$= \lambda(\lambda-1)^{16\times2^{n+1}-29}.\ \left(\frac{\lambda(\lambda-1)^{16}}{\lambda}\right)^{2^{n+1}}$$

$$= \lambda(\lambda-1)^{16\times2^{n+1}-29}.(\lambda-1)^{16\times2^{n+1}}$$

$$= \lambda(\lambda-1)^{16\times2^{n+2}-29}.$$

Corollary 2. (i) The order of $PD_2[n]$ is $|V(PD_2[n])| = 16\times 2^{n+2} - 28.$
(ii) The size of $PD_2[n]$ is $|E(PD_2[n])| = 16\times 2^{n+2} - 29.$

Proof. (i) Using Lemma 1(i), $\deg(P(G,\lambda)) = |V(G)|$. By Theorem 4, $\deg(P(PD_2[n],\lambda)) =$ $16\times 2^{n+2} - 28.$ Therefore $|V(PD_2[n])| = 16\times 2^{n+2} - 28.$
(ii) Using Lemma 1(iii), the coefficient of $\lambda^{|V(G)|-1}$ is the number of edges of *G*. By Theorem 4, $|E(PD_2[n])| = 16\times 2^{n+2} - 29.$

Finally we shall compute another chromatic polynomials of a class dendrimer nanostars by construction of dendrimer generations G_n has grown *n* stages. We denote simply this graph by $DS_1[n]$. Figure 4 shows that generations G_3 has grown 3 stages.

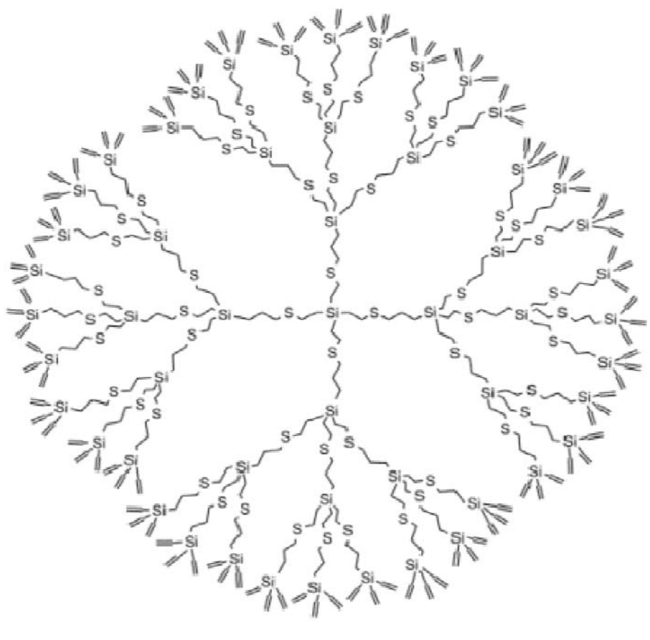

Fig. 4. Dendrimer nanostars of generation G_n has grown 3 stages, $DS_1[n]$

Theorem 5. Let $n \in N_0$. The chromatic polynomial of $DS_1[n]$ is

$$P(DS_1[n],\lambda)=\lambda(\lambda-1)^{2\times 3^{n+2}-14}.$$

Proof. By induction on *n*. Since $P(DS_1[0],\lambda)=\lambda(\lambda-1)^4$, the result is true for *n* = 0. Now suppose that the result is true for less than *n* and we prove it for *n*. Since

$$P(DS_1[n],\lambda)=P(DS_1[n-1]\times\underbrace{(4)S_5}_{4\times 3^{n-1}-times},\lambda),$$

by Theorem 2, we have

$$P(DS_1[n],\lambda)=P(DS_1[n-1])\left(\frac{(\lambda-1)^5}{\lambda}P(S_5,\lambda)\right)^{4\times 3^{n-1}}.$$

Now by induction hypothesis, we have

$$\begin{aligned}P(DS_1[n],\lambda)\ &=\lambda(\lambda-1)^{2\times 3^{n+1}-14}.\left(\frac{(\lambda-1)^5}{\lambda}.\lambda(\lambda-1)^4\right)^{4\times 3^{n-1}}\\ &=\lambda(\lambda-1)^{2\times 3^{n+1}-14}.\ (\lambda-1)^{9\times 4\times 3^{n-1}}\\ &=\lambda(\lambda-1)^{2\times 3^{n+2}-14}.\end{aligned}$$

Corollary 3. (i) The order of $DS_1[n]$ is $|V(DS_1[n])|=2\times 3^{n+2}-13.$
(ii) The size of $DS_1[n]$ is $|E(DS_1[n])|=2\times 3^{n+2}-14.$

Proof. (i) Using Lemma 1(i), $\deg(P(G,\lambda))=|V(G)|$. By Theorem 5, $\deg(P(DS_1[n],\lambda))=2\times 3^{n+2}-13.$ Therefore $|V(DS_1[n])|=2\times 3^{n+2}-13.$
(ii) Using Lemma 1(iii), the coefficient of $\lambda^{|V(G)|-1}$ is the number of edges of *G*. By Theorem 5, $|E(DS_1[n])|=2\times 3^{n+2}-14.$

The following corollary is the immediate conclusion of Theorems 3, 4 and 5.

Corollary 4. The chromatic roots of graphs $PD_1[n]$, $PD_2[n]$ and $DS_1[n]$ are {0,1}.

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