

Article

On chromatic polynomial of certain families of dendrimer graphs

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Abstract: Let G be a simple graph with vertex set $V(G)$ and edge set $E(G)$. A mapping $g : V(G) \rightarrow \{1, 2, \dots, t\}$ is called t -coloring if for every edge $e = (u, v)$, we have $g(u) \neq g(v)$. The *chromatic number* of the graph G is the minimum number of colors that are required to properly color the graph. The chromatic polynomial of the graph G , denoted by $P(G, t)$ is the number of all possible proper coloring of G . 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. In this paper, the chromatic polynomials for certain families of dendrimer nanostars have been computed.

Keywords: t -coloring, chromatic polynomials, dendrimer nanostars.

MSC: 05C12, 05C90.

1. Introduction

A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects known as vertices together with a set $E(G)$ of unordered pairs of distinct vertices of G known as edges. The t -coloring of a graph G is a function $g : V(G) \rightarrow \{1, 2, \dots, t\}$ which satisfies $g(u) \neq g(v)$ for any edge $e = (uv)$. In 1912, Birkhoff [1], presented the concept of *chromatic polynomial* to solve the four color problem. More precisely, a graph G is said to be t -colorable if such t -coloring exists and we say G is t -colorable. The *chromatic number* $\chi(G)$ is the minimal t for which the graph is t -colorable, and we say that G is t -chromatic if $\chi(G) = t$.

The chromatic polynomial is defined as the number of distinct t -colorings in a graph G and is denoted by the $P(G, t)$. If the two graphs G and H have the same chromatic polynomial then the graphs defined as the chromatically equivalent graphs. In recent years, the fields of cheminformatics, physics, computer sciences and other social sciences have attracted their attention for research prospects in graph theory. A lot of research has been done by using concepts of graph theory in these fields. In molecular graphs, the vertices of the graph represent the atoms of the molecule, and the edges represent the chemical bonds.

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 supramolecular chemistry, particularly in host guest reactions and self-assembly processes. Their applications in chemistry, biology and nanoscience are unlimited. Currently, Alikhani *et al.* in [2] investigated the mathematical properties of the nanostructures and some of their chromatic polynomials. In this paper, we have investigated the chromatic polynomials of certain dendrimers nanostars.

2. Known Results

In this section, we present some known result about chromatic polynomials of dendrimer graphs.

Theorem 1. [3] *Fundamental Reduction Theorem.*

$$P(G, t) = P(G - e, t) - P(G/e, t).$$

Suppose that G is a simple graph which has an edge e . Then $G - e$ is a graph obtained from the graph G by eliminating an edge e and G/e is a graph obtained from the graph G by contracting an edge e to one vertex.

Let P_{m+1} be a path with vertices $y_0, y_1, y_2, \dots, y_m$ and G be any graph. The graph $G_{v_0}(m) = G(m)$ is a graph obtained from G by identifying a 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} . The chromatic polynomial of the graph $G(m)$ [2] is:

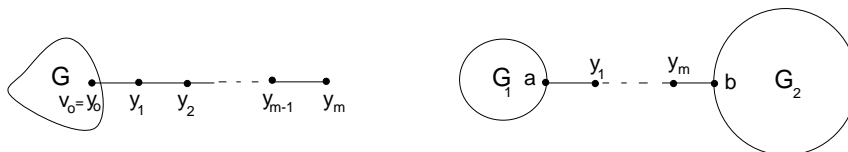


Figure 1. The Graphs $G(m)$ and $G_1(m)G_2$

$$P(G_m, t) = (t - 1)^m P(G, t), \tag{1}$$

and the chromatic polynomial of the graph $G_1(m)G_2$ [2] is:

$$P(G_1(m)G_2, t) = \frac{(t - 1)^{m+1} P(G_1, t) P(G_2, t)}{t}. \tag{2}$$

Theorem 2. [4] If the graphs G and H have only one common vertex, such that $V(G) \cup V(H) = v$, we have

$$P(G \cup H, t) = \frac{P(G, t) P(H, t)}{t}.$$

Lemma 3. [5] Let G be a graph of order n and size m and $P(G, t)$ be the chromatic polynomial of G , then

- a) $\deg(P(G, t)) = n$,
- b) the coefficient of t^n is 1,
- c) the coefficient of t^{n-1} is $-m$.

3. Main Results

3.1. Chromatic polynomial of Polyaryl Ether dendrimer

Polyaryl ether dendrimer is an important class of commercial polymers. The 32 carboxylate groups on dendrimers surface makes it highly soluble in basic aqueous solution, its three dimensional structure is constructed in possessing a central unit or core unit denoted by $G_1(0)$ (see Figure 2). Its branches, also known as added branches which are denoted by the graph H (see Figure 3) and the end groups which overall has grown to n number of stages. The graph can be divided into 4^n hexagonal in each step. The graph of polyaryl ether dendrimer is denoted by $G_1(n)$ and shown in the Figure 4.

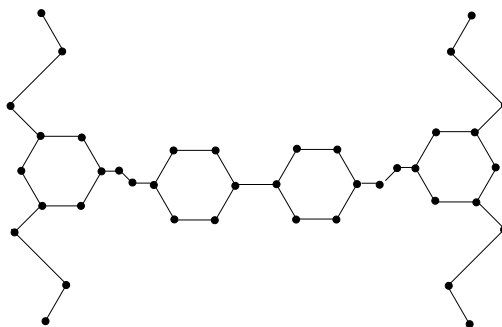


Figure 2. The graph of polyaryl ether dendrimer nanostar $G_1(0)$

The following two theorems presents the formula for chromatic polynomial of the $G_1(0)$ and $G_1(n)$.

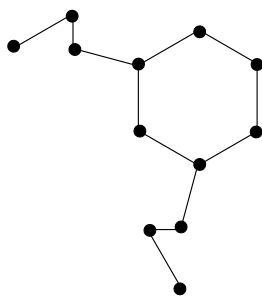


Figure 3. The graph of added branch of polyaryl ether dendrimer nanostar denoted by H .

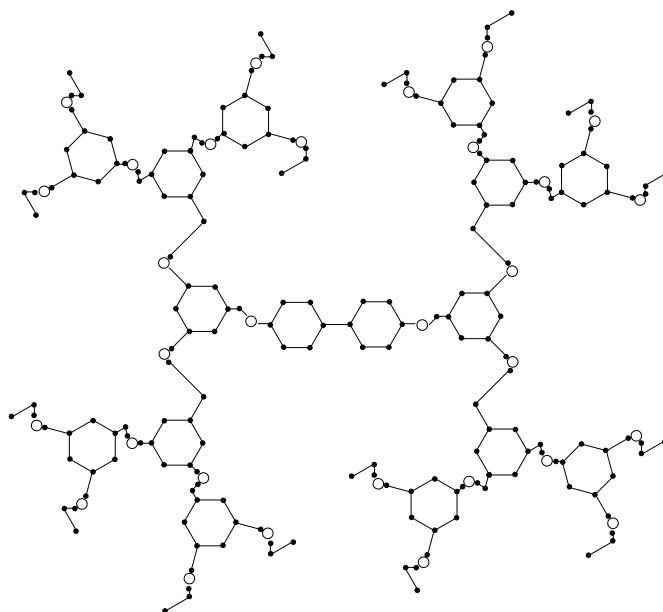


Figure 4. The graph of polyaryl ether dendrimer $G_1(2)$

Theorem 4. The chromatic polynomial of the polyaryl ether dendrimer $G_1(0)$ is

$$P(G_1(0), t) = t(t - 1)^{23}(t^4 - 5t^3 + 10t^2 - 10t + 5)^4.$$

Proof. By applying Theorem 2 and Equation (1), we get

$$P(G_1(0), t) = \frac{(t - 1)^{19}(P(C_6, t))^4}{t^3} = t(t - 1)^{23}(t^4 - 5t^3 + 10t^2 - 10t + 5)^4.$$

□

Theorem 5. For $n \geq 0$, the chromatic polynomial of $G_1(n)$ is as:

$$P(G_1(n), t) = t(t - 1)^{28 \cdot 2^n - 5}(t^4 - 5t^3 + 10t^2 - 10t + 5)^{2^{n+2}}.$$

Proof. The proof is constructed by induction on n . Since result is true for $n = 0$ by Theorem 4. Let us suppose that the result is true for any values less than n and we prove it for n . The chromatic polynomial of core of polyaryl ether dendrimer graph is

$$P(G_1(0), t) = t(t - 1)^{23}(t^4 - 5t^3 + 10t^2 - 10t + 5)^4.$$

The chromatic polynomial of the graph H is computed by applying Theorem 2 and Equation (1).

$$P(H, t) = (t - 1)^6 P(C_6, t) = P(H, t) = t(t - 1)^7(t^4 - 5t^3 + 10t^2 - 10t + 5),$$

For $n \geq 1$, the graph $G_1(n)$ is obtained from $G_1(n - 1)$ by adding $4(2)^{n-1}$ copies of the graph H such that each copy of the graph H has vertex in common with the graph $G_1(n - 1)$. Therefore by Theorem 2 we get,

$$P(G_1(m), t) = \frac{P(G_1(m - 1), t) \times (P(H, t))^{4(2^{m-1})}}{t^{4(2^{m-1})}}, \quad 1 \leq m \leq n.$$

Now by using the backward substitution, we get

$$\begin{aligned} P(G_1(n), t) &= \frac{P(G_1(0), t) \times (P(H, t))^{4(2^{n-1})}}{t^{4(2^{n-1})}} \\ &= \frac{t(t - 1)^{23}(t^4 - 5t^3 + 10t^2 - 10t + 5)^4(t(t - 1))^7(t^4 - 5t^3 + 10t^2 - 10t + 5)^{4(2^{n-1})}}{t^{4(2^{n-1})}}. \end{aligned}$$

Hence we conclude that

$$P(G_1(n), t) = t(t - 1)^{28(2^n)-5}(t^4 - 5t^3 + 10t^2 - 10t + 5)^{2^{n+2}}.$$

□

The following result presents the formula for order and size of the Polyaryl ether dendrimer nanostar $G_1(n)$.

Corollary 6. Let $G_1(n)$ be the polyaryl ether dendrimer nanostar. Then

- a) $|V(G_1(n))| = 44(2^n) - 4,$
- b) $|E_{G_1(n)}| = 48(2^n) - 5.$

Proof. a) Using Lemma 3(a), $deg(P(G, t)) = |V(G)|$ which states that the degree of the chromatic polynomials is equal to the number of vertices in that graph. Since, $deg(P(G_1(n), t)) = 44(2^n) - 4$ therefore by the Theorem 5, we get

$$|V(G_1(n))| = 44(2^n) - 4.$$

b) Using Lemma 3(c), the coefficient of $-t^{|V(G)-1}|$ is equal with the number of edges of G . So, Theorem 5 implies that

$$|E(G_1(n))| = 48(2^n) - 5.$$

□

3.2. Chromatic polynomial of Organosilicon dendrimer

The organosilicon dendrimers was first studied and prepared by Nakayama and Lin [?]. Organosilicon dendrimer graph denoted by $G[n]$ which is different by its construction consisting of three major parts, the core unit denoted by $G[1]$ (Figure 5), added branches which is denoted by the graph H and the end groups which overall has grown to n stages. Let H_1 is the graph obtained by vertex gluing of C_5 and K_2 . The graph H is obtained by vertex gluing of 3 copies of H_1 and path P_2 . The graph can be divided into $6(3^{n-1}) - 2$ pentagons in each stage. The graph H and $G[2]$ is shown in Figures 6 and 7.

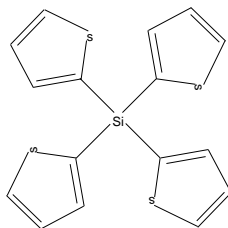


Figure 5. The graph of organosilicon dendrimer $G[1]$

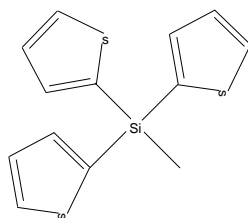


Figure 6. The graph of added branch of organosilicon dendrimer H

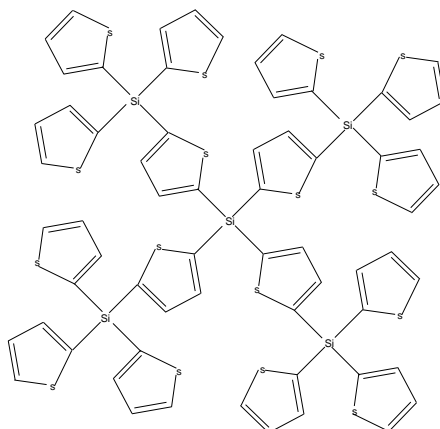


Figure 7. The graph of organosilicon dendrimer $G[2]$

The following three theorems presents the formula for chromatic polynomial of the Organosilicon dendrimer $G[1]$, $G[2]$ and $G[n]$.

Theorem 7. *The chromatic polynomial of Organosilicon dendrimer $G[1]$ is*

$$P(G[1], t) = t(t - 1)^8(t^3 - 4t^2 + 6t - 4)^4.$$

Proof. By applying Theorem 2, we get

$$P(H_1, t) = \frac{P(C_5, t)P(K_2, t)}{t} = (t - 1)((t - 1)^5 - (t - 1)) = t(t - 1)^2(t^3 - 4t^2 + 6t - 4).$$

Since, the graph $G[1]$ is composed of 4 copies of the graph H_1 such that each copy of the H_1 intersect at the common vertex t , where $t = Si$ from Figure 5. Therefore, from Theorem 2, we have

$$P(G[1], t) = \frac{P(H_1, t)P(H_1, t)P(H_1, t)P(H_1, t)}{t.t.t} = \frac{t^4(t - 1)^8(t^3 - 4t^2 + 6t - 4)^4}{t^3},$$

This implies that,

$$P(G[1], t) = t(t - 1)^8(t^3 - 4t^2 + 6t - 4)^4.$$

□

Theorem 8. *For $n \geq 1$, the chromatic polynomial of $G[n]$ is*

$$P(G[n], t) = t(t - 1)^{14(3^{n-1})-6}(t^3 - 4t^2 + 6t - 4)^{6(3^{n-1})-2}.$$

Proof. The proof is constructed by induction on n . Since the result is true for $n = 1$ by Theorem 7. Let us suppose that the result is true for any values less than n and we prove it for n . The chromatic polynomial of organosilicon dendrimer for $G[1]$ is,

$$P(G[1], t) = t(t-1)^8(t^3 - 4t^2 + 6t - 4)^4.$$

The chromatic polynomial of Organosilicon dendrimer for the graph H can be computed by applying Theorem 2 and Equation (1), as follows

$$P(H, t) = \frac{(t-1)^4(P(C_5, t))^3}{t^2} = t(t-1)^7(t^3 - 4t^2 + 6t - 4)^3.$$

For $n \geq 2$, the graph $G[n]$ is obtained from $G[n-1]$ by adding $4(3)^{n-2}$ copies of the graph H such that each copy of the graph H has vertex in common with the graph $G[n-1]$. Therefore by Theorem 2, we get

$$P(G[m], t) = \frac{P(G[m-1], t) \times (P(H, t))^{4(3^{m-2})}}{t^{4(3^{m-2})}}, \quad 2 \leq m \leq n.$$

Now by using the backward substitution, we get

$$\begin{aligned} P(G[n], t) &= \frac{P(G[1], t) \times (P(H, t))^{2(3^{n-1}-1)}}{t^{2(3^{n-1}-1)}} \\ &= t(t-1)^8(t^3 - 4t^2 + 6t - 4)^4((t-1)^7(t^3 - 4t^2 + 6t - 4))^{2(3^{n-1}-1)} \\ &= t(t-1)^{14(3^{n-1})-6}(t^3 - 4t^2 + 6t - 4)^{6 \times 3^{n-1}-2}. \end{aligned}$$

□

The following result presents the formula for order and size of the Organosilicon dendrimer $G[n]$.

Corollary 9. For the Organosilicon dendrimer $G[n]$, we have

- a) $|V(G[n])| = 21 + 32[3^{n-1} - 1]$,
- b) $|E(G[n])| = 24 + 38[3^{n-1} - 1]$.

Proof. a) Using Lemma 3(a), $\deg(P(G, t)) = |V(G)|$ which states that the degree of the chromatic polynomial is equal to the number of vertices in that graph. Since, $\deg(P(G, t)) = 21 + 32[3^{n-1} - 1]$, therefore Theorem 8 implies that

$$|V(G[n])| = 21 + 32[3^{n-1} - 1].$$

b) Using Lemma 3(c), the coefficient of $-t^{|V(G)-1|}$ is equal with the number of edges of G . So Theorem 8 implies that

$$|E(G[n])| = 24 + 38[3^{n-1} - 1].$$

□

3.3. Chromatic polynomial of Nanostar dendrimer

For $n \geq 1$, the graph of Nanostar dendrimer NSC_5C_6 denoted by $G_2(n)$ which is different by its construction consisting of major parts core unit, added branches and end groups, which overall has grown to n stages. First stage consists of a hexagon with two pentagons and for $n \geq 2$ the new branches $4(2^{n-2})$ emitting from the very first stage are added and their step wise growth follows a structure of Nanostar dendrimer NSC_5C_6 . The graph of $G_2(2)$ and the graph of added branch denoted by H is shown in Figures 8 and 9 respectively. Now, we will determine the chromatic polynomial of family of dendrimer nanostar NSC_5C_6 denoted by $G_2(n)$.

The following two theorems presents the formula for chromatic polynomial of the $G_2(1)$ and $G_2(n)$.

Theorem 10. The chromatic polynomial of Nanostar dendrimer NSC_5C_6 denoted by $G_2(1)$ is:

$$P(G_2(1), t) = t(t-1)^{17}(t^3 - 4t^2 + 6t - 4)^2(t^4 - 5t^3 + 10t^2 - 10t + 5).$$

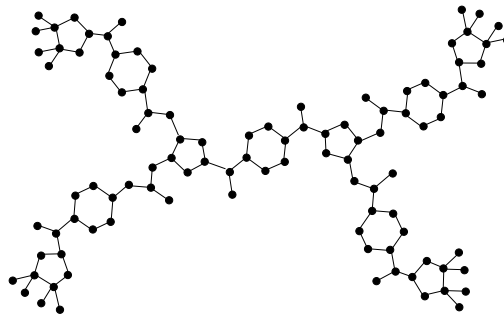


Figure 8. The graph $G_2(2)$ of dendrimer nanostar NSC_5C_6

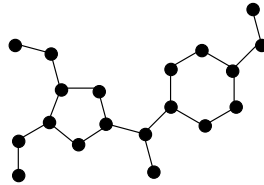


Figure 9. The graph H of added branch of dendrimer nanostar NSC_5C_6

Proof. By applying Theorem 2 and Equation (1), we get

$$P(G_2(1), t) = \frac{(t - 1)^{14}P(C_6, t)(P(C_5, t))^2}{t^2} = t(t - 1)^{17}(t^3 - 4t^2 + 6t - 4)^2(t^4 - 5t^3 + 10t^2 - 10t + 5).$$

□

Theorem 11. For $n \geq 0$, the chromatic polynomial of $G_2(n)$ is:

$$P(G_2(n), t) = t(t - 1)^{11(2^{n+1})-27}(t^3 - 4t^2 + 6t - 4)^{2^{n+1}-2}(t^4 - 5t^3 + 10t^2 - 10t + 5)^{2^{n+1}-3}.$$

Proof. The proof is constructed by induction on n . Since the result is true for $n = 1$ by Theorem 10. Let us suppose that the result is true for any values less than n and we prove it for n . The chromatic polynomial of $G_2(1)$ is

$$P(G_2(1), t) = t(t - 1)^{17}(t^3 - 4t^2 + 6t - 4)^2(t^4 - 5t^3 + 10t^2 - 10t + 5).$$

The chromatic polynomial for the graph H can be calculated by applying Theorem 2 and Equation (1), we get

$$P(H, t) = \frac{(t - 1)^9P(C_5, t)P(C_6, t)}{t} = t(t - 1)^{11}(t^3 - 4t^2 + 6t - 4)(t^4 - 5t^3 + 10t^2 - 10t + 5).$$

For $n \geq 2$, the graph $G_2(n)$ is obtained from $G_2(n - 1)$ by adding $4(2)^{n-2}$ copies of the added graph H such that each copy of the graph H has vertex in common with the graph $G_2(n - 1)$. Therefore by Theorem 2, we get

$$P(G_2(m), t) = \frac{P(G_2(m - 1), t) \times (P(H, t))^{4(2^{m-2})}}{t^{4(2^{m-2})}}, \quad 2 \leq m \leq n.$$

Now by using the backward substitution, we get

$$\begin{aligned} P(G_2(n), t) &= \frac{P(G_2(1), t) \times (P(H, t))^{4(2^{n-1}-1)}}{t^{4(2^{n-1}-1)}} \\ &= t(t - 1)^{17}(t^3 - 4t^2 + 6t - 4)^2(t^4 - 5t^3 + 10t^2 - 10t + 5) \\ &\quad \times [(t - 1)^{11}(t^3 - 4t^2 + 6t - 4)(t^4 - 5t^3 + 10t^2 - 10t + 5)]^{4(2^{n-1}-1)}. \end{aligned}$$

Hence we conclude that

$$P(G_2(n), t) = t(t - 1)^{11(2^{n+1})-27}(t^3 - 4t^2 + 6t - 4)^{2^{n+1}-2}(t^4 - 5t^3 + 10t^2 - 10t + 5)^{2^{n+1}-3}.$$

□

The following result presents the formula for order and size of the Nanostar dendrimer.

Corollary 12. Let $G_2(n)$ be the Nanostar dendrimer NSC_5C_6 . Then we have

- a) $|V(G_2(n))| = 9 \times 2^{n+2} - 44,$
- b) $|E(G_2(n))| = 9 \times 2^{n+2} - 45.$

Proof. a) Using Lemma 3(a), $deg(P(G, t)) = |V(G)|$ which states that the degree of the chromatic polynomial is equal to the number of vertices in that graph. Since, $deg(P(G_2(n), t)) = 9 \times 2^{n+2} - 44,$ therefore Theorem 11 implies that,

$$|V(G_2(n), t)| = 9 \times 2^{n+2} - 44.$$

b) Using Lemma 3 (c), the coefficient of $-t^{|V(G)-1}|$ is equal with the number of edges of G . So Theorem 11 implies that

$$|E(G_2(n), t)| = 9 \times 2^{n+2} - 45.$$

□

3.4. Chromatic polynomial of Tetrathiafulvalence dendrimer

The graph of Tetrathiafulvalence dendrimer simply denoted by $TD_2[n]$ consisting of core unit, added branches and end groups which has overall grown to n stages and each stage consists of $2^{n+3} - 6$ pentagons with $2^{n+3} - 4$ hexagons. After the core unit stage, for $n \geq 1, 4(2^{n-1})$ branches are added to every stage of the graph and hence, their stepwise growth follows a structure of the tetrathiafulvalence dendrimer, $TD_2[n]$. The graph of $TD_2[0]$ is the core of graph, the graph of added branch H and the graph of $TD_2[1]$ is shown in Figure 10, 11 and 12. Now, we will determined the chromatic polynomial of class of dendrimer known as tetrathiafulvalence dendrimer $TD_2[n]$.

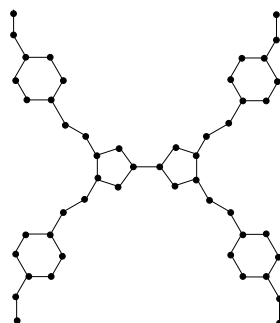


Figure 10. The core of tetrathiafulvalence dendrimer $TD_2[0]$.

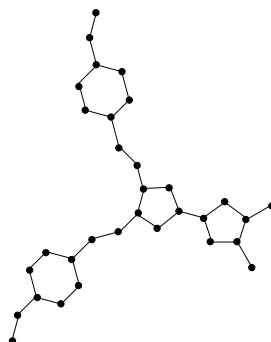


Figure 11. The added graph H in each branch of $TD_2[n]$.

The following two theorems presents the formula for chromatic polynomial of $TD_2[0]$ and $TD_2[n]$.

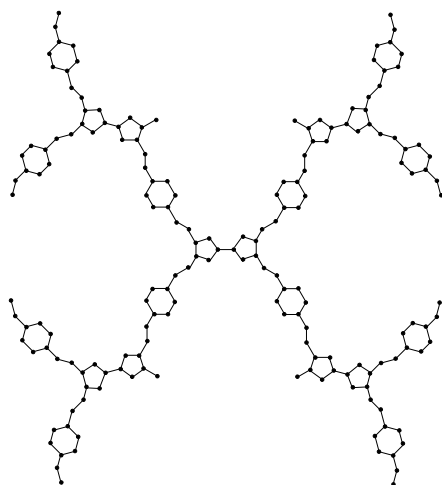


Figure 12. The graph of Tetrathiafulvalence dendrimer, $TD_2[1]$.

Theorem 13. The chromatic polynomial of tetrathiafulvalence dendrimer $TD_2[0]$ is:

$$P(TD_2[0], t) = t(t-1)^{27}(t^3 - 4t^2 + 6t - 4)^2(t^4 - 5t^3 + 10t^2 - 10t + 5)^4.$$

Proof. By applying Theorem 2 and Equation (1), we get

$$P(TD_2[0], t) = \frac{(t-1)^{21}(P(C_6, t))^4(P(C_5, t))^2}{t^5}.$$

This implies that

$$P(TD_2[0], t) = t(t-1)^{27}(t^3 - 4t^2 + 6t - 4)^2(t^4 - 5t^3 + 10t^2 - 10t + 5)^4.$$

□

Theorem 14. For $n \geq 0$, the chromatic polynomial of $TD_2[n]$ is:

$$P(TD_2[n], t) = t(t-1)^{17(2^{n+2})-41}(t^3 - 4t^2 + 6t - 4)^{2^{n+3}-6}(t^4 - 5t^3 + 10t^2 - 10t + 5)^{2^{n+3}-4}.$$

Proof. The proof is constructed by induction on n . Since the result is true for $n = 0$ by Theorem 13. Let us suppose that the result is true for any values less than n and we prove it for n . The chromatic polynomial of the graph $TD_2[n]$ is

$$P(TD_2[0], t) = t(t-1)^{27}(t^3 - 4t^2 + 6t - 4)^2(t^4 - 5t^3 + 10t^2 - 10t + 5)^4.$$

The chromatic polynomial for graph H can be calculated by applying Theorem 2 and Equation (1), as follows:

$$P(H, t) = \frac{(t-1)^{13}(P(C_6, t))^2(P(C_5, t))^2}{t^3} = t(t-1)^{17}(t^3 - 4t^2 + 6t - 4)^2(t^4 - 5t^3 + 10t^2 - 10t + 5)^2.$$

For $n \geq 1$, the graph $TD_2[n]$ is obtained from $TD_2[n-1]$ by adding $4(2)^{n-1}$ copies of the graph H such that each copy of the graph H has vertex in common with the graph $TD_2[n-1]$. Therefore by Theorem 2, we have

$$P(TD_2[m], t) = \frac{P(TD_2[m-1], t) \times (P(H, t))^{4(2^{m-1})}}{t^{4(2^{m-1})}}, \quad 1 \leq m \leq n.$$

Now by using the backward substitution, we get

$$\begin{aligned}
 P(TD_2[n], t) &= \frac{P(TD_2[0], t) \times (P(H, t))^{4(2^n-1)}}{t^{4(2^n-1)}} \\
 &= \frac{t(t-1)^{27}(t^3-4t^2+6t-4)^2(t^4-5t^3+10t^2-10t+5)^4}{t^{4(2^n-1)}} \\
 &\quad \times \frac{[t(t-1)^{17}(t^3-4t^2+6t-4)^2(t^4-5t^3+10t^2-10t+5)^2]^{4(2^n-1)}}{t^{4(2^n-1)}}.
 \end{aligned}$$

Hence we conclude that

$$P(TD_2[n]), t) = t(t-1)^{17(2^{n+2})-41}(t^3-4t^2+6t-4)^{2^{n+3}-6}(t^4-5t^3+10t^2-10t+5)^{2^{n+3}-4}.$$

□

The following result presents the formula for size and order of Tetrathiafulvalence dendrimer.

Corollary 15. For the Tetrathiafulvalence dendrimer $TD_2[n]$, we have

- a) $|V(TD_2[n])| = 50 + 124(2^n - 1),$
- b) $|E(TD_2[n])| = 5(28(2^n) - 17).$

Proof. a) Using Lemma 3(a), $deg(P(G, t)) = |V(G)|$ which states that the degree of the chromatic polynomial is equal to the number of vertices in that graph. Since, $deg(P(TD_2[n], t)) = 50 + 124(2^n - 1),$ therefore Theorem 14 implies that

$$|V(TD_2[n], t)| = 50 + 124(2^n - 1).$$

b) Using Lemma 3(c), the coefficient of $-t^{|V(G)-1}|$ is equal with the number of edges of $G.$ So Theorem 14 implies that

$$|E(TD_2[n], t)| = 5(28(2^n) - 17).$$

□

3.5. Chromatic polynomial of Polyther nanostar dendrimer

The graph of polyther dendrimer $PD_3[n]$ consisting of core unit, added branches and end groups which has overall grown to the n stages and each stage consists of $3(2^{n+1} - 1)$ hexagons. The new branches $3(2^n - 1)$ emitting from the very first stage are added and their step wise growth follows a structure of polyther dendrimer nanostar $PD_3[n].$ The core of polyther dendrimer $PD_3[0]$ and the graph of $PD_3[1]$ and the graph of added branch H is shown in Figure 13, 14 and 15.

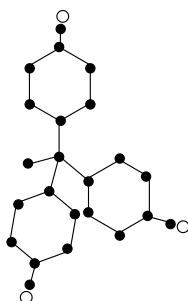


Figure 13. The core of polyther dendrimer $PD_3[0].$

Now, we will determine the chromatic polynomial of family of Polyther nanostar dendrimer $PD_3[n].$

The following three theorems presents the chromatic polynomial of the Polyther nanostar dendrimer $PD_3[0]$ and $PD_3[n].$

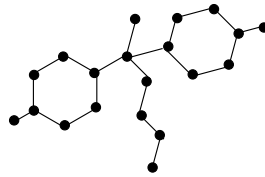


Figure 14. The graph of H of polyther dendrimer $PD_3[n]$.

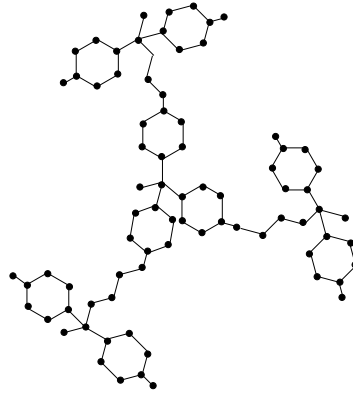


Figure 15. The graph of polyther dendrimer $PD_3[1]$.

Theorem 16. The chromatic polynomial of polyther dendrimer nanostar $PD_3[0]$ is

$$P(PD_3[0], t) = t(t - 1)^{10}(t^4 - 5t^3 + 10t^2 - 10t + 5)^3.$$

Proof. By applying Theorem 2 and Equation (1), we get

$$P(PD_3[0], t) = \frac{(t - 1)^7(P(C_6, t))^3}{t^2}.$$

This implies that

$$P(PD_3[0], t) = t(t - 1)^{10}(t^4 - 5t^3 + 10t^2 - 10t + 5)^3.$$

□

Theorem 17. For $n \geq 0$, the chromatic polynomial of $PD_3[n]$ is:

$$P(PD_3[n], t) = t(t - 1)^{33(2^n) - 23}(t^4 - 5t^3 + 10t^2 - 10t + 5)^{3(2^{n+1}) - 3}.$$

Proof. The proof is constructed by induction on n . Since the result is true for $n = 0$ by Theorem 16. Let us suppose that the result is true for any values less than n and we prove it for n . The chromatic polynomial of polyther dendrimer for $PD_3[1]$ is

$$P(PD_3[0], t) = t(t - 1)^{10}(t^4 - 5t^3 + 10t^2 - 10t + 5)^3.$$

The chromatic polynomial for the graph H can be calculated by applying Theorem 2 and Equation (1), we get

$$P(H, t) = \frac{(t - 1)^9(P(C_6, t))^2}{t} = t(t - 1)^{11}(t^4 - 5t^3 + 10t^2 - 10t + 5)^2.$$

For $n \geq 1$, the graph $PD_3[n]$ is obtained from $PD_3[n - 1]$ by adding $3(2)^{n-1}$ copies of the added graph H such that each copy of the graph H has vertex in common with the graph $PD_3[n - 1]$. Therefore by Theorem 2, we get

$$P(PD_3[m], t) = \frac{P(PD_3[m - 1], t) \times (P(H, t))^{3(2^{m-1})}}{t^{3(2^{m-1})}}, \quad 1 \leq m \leq n.$$

Now by using the backward substitution, we get

$$P(PD_3[n], t) = t(t-1)^{10}(t^4 - 5t^3 + 10t^2 - 10t + 5)^3 \left[\frac{(t(t-1)^{11}(t^4 - 5t^3 + 10t^2 - 10t + 5)^2)^{3(2^n-1)}}{t^{3(2^n-1)}} \right].$$

Hence we conclude that

$$P(PD_3[n], t) = t(t-1)^{33(2^n)-23}(t^4 - 5t^3 + 10t^2 - 10t + 5)^{3(2^{n+1})-3}.$$

□

The following result presents the formula for order and size of the polyther dendrimer $PD_3[n]$.

Corollary 18. For the Polyther dendrimer $PD_3[n]$, we have

- a) $|V(PD_3[n])| = 57(2^n) - 34$,
- b) $|E(PD_3[n])| = 63(2^n) - 38$.

Proof. a) Using Lemma 3(a), $\deg(P(G, t)) = |V(G)|$, which states that the degree of the chromatic polynomial is equal to the number of vertices in that graph. Since, $\deg(P(PD_3[n], t)) = 57(2^n) - 34$, therefore Theorem 17 implies that

$$|V(PD_3[n])| = 57(2^n) - 34.$$

b) Using Lemma 3(c), the coefficient of $-t^{|V(G)-1|}$ is equal with the number of edges of G. So Theorem 17 implies that

$$|E(PD_3[n])| = 63(2^n) - 38.$$

□

4. Conclusion

Dendrimers have wide range of applications in supra-molecular chemistry, particularly in host guest reactions and self-assembly processes. During the past several years, there are many research papers dealing with the study of mathematical and topological properties of certain dendrimer nano-structures in [6–10]. Currently, Alikhani and Iranmanesh investigated the mathematical properties of the nanostructures and some of their chromatic polynomials [2]. In this paper, we have extended this study and computed the chromatic polynomials of certain dendrimers.

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