

PACKING CHROMATIC NUMBER OF CERTAIN DENDRIMERS

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Abstract: The packing chromatic number $\chi_\rho(G)$ of a graph G is the smallest integer k for which there exists a mapping $f : V(G) \rightarrow \{1, 2, \dots, k\}$ such that any two vertices of color i are at distance at least $i + 1$. In bio-chemistry, dendrimers are synthetically produced monodisperse polymeric nanostructures with a tree-like, highly branched architecture. Applications of dendrimers typically involve conjugating other chemical species to the dendrimer surface that can function as detecting agents, affinity ligands, targeting components, radioligands, imaging agents, or pharmaceutically active compounds. In this paper, the packing chromatic number of certain dendrimers $D_{2,k}$, $k = 1, 2, 3, 4$ are calculated. We also post some open problems.

AMS Subject Classification: 05C15

Key Words: packing coloring, bethe tree, dendrimer

1. Introduction

Let G be a connected graph and k be an integer, $k \geq 1$. A packing k -coloring of a graph G is a mapping $f : V(G) \rightarrow \{1, 2, \dots, k\}$ such that any two vertices of color i are at distance at least $i + 1$. The packing chromatic number $\chi_\rho(G)$ of G is the smallest integer k for which G has packing k -coloring. The concept of packing coloring comes from the area of frequency assignment in wireless networks and was introduced by Goddard et al. [2] under the name Broad-

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cast coloring. It also has several applications, such as, resource placement and biological diversity. The term packing chromatic number was introduced by Bresar [1].

Dendrimers are novel synthetic polymeric systems having improved physical and chemical properties due to their unique three dimensional architecture. Dendrimers have a well defined size, shape, molecular weight and monodispersity. These are compatible with drug moieties as well as bioactive molecules like DNA, heparin and other polyanions [5]. In this paper, we calculate the packing chromatic number of certain class of dendrimers.

2. Main Results

Proposition 1. [2] *Let H be a subgraph of G . Then $\chi_\rho(H) \leq \chi_\rho(G)$.*

Proposition 2. [2] *Let C_n be a cycle on n vertices. Then $\chi_\rho(C_n) = 4$ when n is not a multiple of 4.*

Definition 3. [4] *The Bethe tree $B_{d,k}$ is the rooted tree of k levels whose root vertex has degree d , the vertices from level 2 to level $k - 1$ have degree $d + 1$ and the vertices at level k have degree 1.*

Mahdieh Azari et al. [3] introduced a class of dendrimers which is constructed from copies of ordinary Bethe trees. This molecular structure can be encountered in real chemistry, e.g. in some tertiary phosphine dendrimers. Let D_0 be the graph depicted in Figure 1(a). For $d, k > 0$, let $D_{d,k}$ be a series of dendrimers obtained by attaching d pendent vertices to each pendent vertex of $D_{d,k-1}$ and let $D_{d,0} = D_0$. The diameter of $D_{d,k}$ is $2(d + k)$.

In the following Theorems, $c(v)$ and $d(u, v)$ denote the color of a vertex v and distance between vertices u and v respectively.

Theorem 4. *For D_0 , $\chi_\rho(D_0) = 4$.*

Proof. Since C_6 is a subgraph of D_0 , by Propositions 1 and 2, $\chi_\rho(D_0) \geq 4$. And from Figure 1(a), $\chi_\rho(D_0) = 4$. \square

Theorem 5. *For $D_{2,1}$, $\chi_\rho(D_{2,1}) = 5$.*

Proof. Suppose for the sake of contradiction that this is not true. Then $\chi_\rho(D_{2,1}) = 4$. Label $D_{2,1}$ as it is shown in Figure 1(b). By degree sequence, the vertices of $D_{2,1}$ can be divided into three sets namely $X = \{a_1, a_2, v_1, v_2\}$, $Y = \{b_1, b_2, v_3, v_4\}$ and $Z = \{c_1, c_2, v_5, v_6\}$ and by assumption atmost one

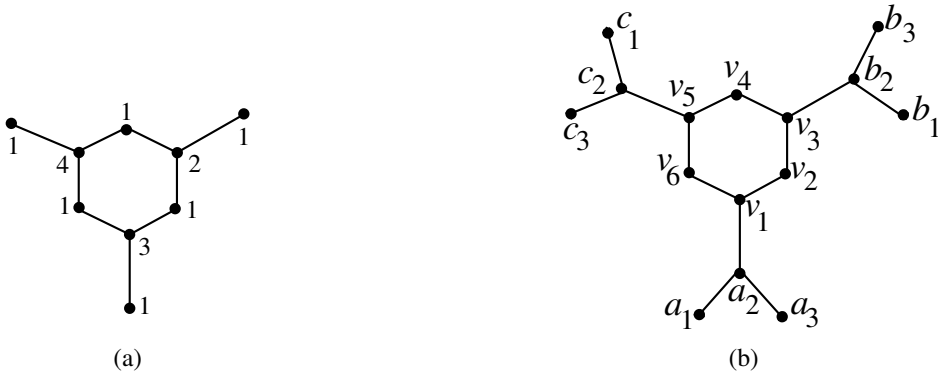


Figure 1: (a) Packing coloring of D_0 . (b) Labelling of $D_{2,1}$

vertex of these sets should receive color 4. Considering the set X for the discussion, it holds true for other vertices in the sets Y and Z due to their degree sequence. Our aim is to minimize the packing coloring. Therefore, we try to label maximum vertices with minimum colors.

Case I: when $c(a_1) = 4$, let $c(a_2) = 1$, $c(v_1) = 3$ and $c(a_3) = 2$. Since $d(a_2, \{v_2, v_6\}) = 2$ and $d(v_2, v_6) = 2$, $c(v_2) = c(v_6) = 1$. Since $d(a_3, v_3) = 4$, $c(v_3) = 2$. Now for vertex v_5 , the only hope is to get a color greater than 4.

Case II: when $c(a_2) = 4$, let $c(a_1) = c(v_1) = c(a_3) = 1$. Since $d(v_1, \{v_3, v_5\}) = 2$ and $d(v_3, v_5) = 2$, $c(v_3) = c(v_5) = 1$. Now, vertices v_2 and v_6 can be colored 2 and 3 respectively. Since vertex v_3 is colored 1, $d(v_4, \{v_2, v_6\}) = 2$ and $d(a_2, v_4) = 4$, the vertex v_3 should receive a color greater than 4.

Case III: when $c(v_1) = 4$, let $c(v_1) = c(v_2) = c(a_2) = 1$. Since $d(v_2, \{v_4, b_2\}) = 2$ and $d(v_4, b_2) = 2$, $c(v_4) = c(b_2) = 1$. Now, vertices a_1 and a_3 can only be colored with 2 and 3 respectively. Since $d(a_3, \{v_5, b_3\}) \geq 4$ and $d(v_5, b_3) = 4$, $c(v_5) = c(b_3) = 3$. Now for vertex b_1 , the only possibility is to get a color greater than 4.

Case IV: when $c(v_2) = 4$, let $c(v_1) = 1$, $c(v_3) = 1$ and $c(a_2) = 2$. Since vertices a_1, a_3, b_1, b_3 and v_5 are at distance ≥ 2 to each other, $c(a_1) = c(a_3) = c(b_1) = c(b_3) = c(v_5) = 1$. Now the vertex v_6 can receive color 2 or 3 but let $c(v_6) = 3$. Since $d(v_6, b_2) = 4$ and $d(a_2, v_4) \geq 3$, $c(b_2) = 3$ and $c(v_4) = 2$. For the vertex c_2 , the vertices received colors 2, 3, 4 are at distance ≤ 2 , at distance ≤ 3 , at distance ≤ 4 respectively and $c(v_5) = 1$. Thus, the vertex c_2 should receive a color greater than 4.

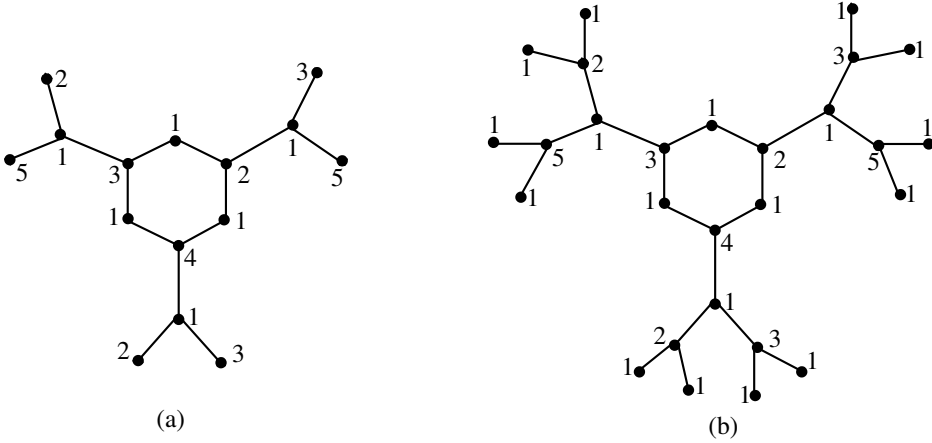


Figure 2: (a) Packing coloring of $D_{2,1}$. (b) Packing coloring of $D_{2,2}$

Hence from above four Cases, $\chi_\rho(D_{2,1}) \geq 5$. From Figure 2(a), we conclude that $\chi_\rho(D_{2,1}) = 5$. □

Theorem 6. For $D_{2,2}$, $\chi_\rho(D_{2,2}) = 5$.

Proof. Since $D_{2,1}$ is a subgraph of $D_{2,2}$, by Propositions 1 and 2, $\chi_\rho(D_{2,2}) \geq 5$. And from Figure 2(b), $\chi_\rho(D_{2,2}) = 5$. □

Theorem 7. For $D_{2,3}$ and $D_{2,4}$, $5 \leq \chi_\rho(D_{2,3}), \chi_\rho(D_{2,4}) \leq 6$.

Proof. Since $D_{2,2}$ is a subgraph of $D_{2,3}$ and $D_{2,4}$, by Propositions 1 and 2, $\chi_\rho(D_{2,3}) \geq 5$ and $\chi_\rho(D_{2,4}) \geq 5$. And from Figures 3(a) and 3(b), $\chi_\rho(D_{2,3}) \leq 6$ and $\chi_\rho(D_{2,4}) \leq 6$. □

3. Open Problems

Problem 1. Determining $\chi_\rho(D_{2,k})$ for $k > 4$ is challenging and the problem remains open.

Problem 2. $\chi_\rho(D_{2,k}) \leq 2(d + k)$.

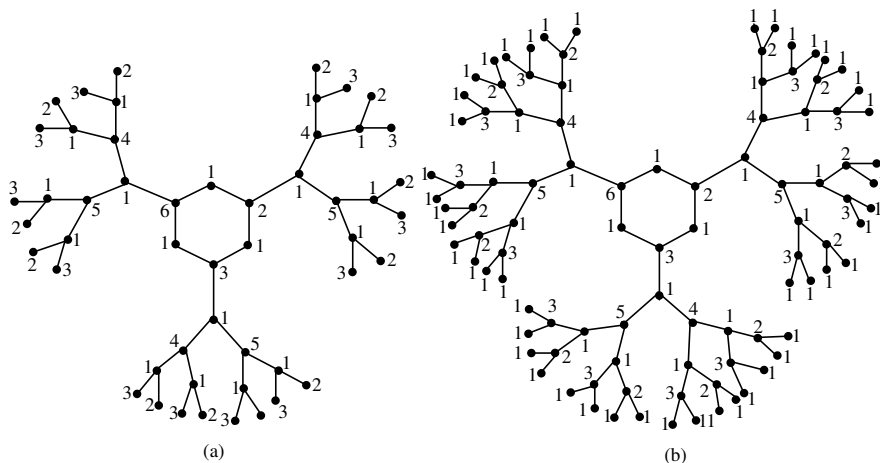


Figure 3: (a) Packing coloring of $D_{2,3}$ (b) Packing coloring of $D_{2,4}$

4. Conclusion

In this paper the packing chromatic number of $D_{2,k}$ for $k = 1, 2, 3, 4$ is calculated and the problem of packing coloring for other chemical structures is under investigation.

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