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Research Paper

Acyclic Coloring of Certain Chemical Structures

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Abstract

A rapidly developing field of science and technology is nanobiotechnology. Nanotube, nanostar and polyomino chain are critical and widespread molecular structures extensively used in the domains of pharmaceuticals, chemical engineering, and medical science. Additionally, these structures serve as the foundational building blocks for other, more intricate chemical molecular structures. In this paper, certain chemical structures like nanostar dendrimer, oxide network, silicate network, boron nanosheet and polyomino chains have been acyclically colored using the concept of vertex cut and matching. Also, we determine the acyclic coloring parameters for the networks under consideration and find a relation between them.

1 Introduction

Nanobiotechnology is an advancing area that uses nanofabrication tools to create devices for studying biological systems. In this field of study, dendrimers are commercially available building blocks. They have a three-dimensional architecture consisting of a core, branches and end groups that is regular and highly branched forming a tree-like structure [1]. The biological characteristics of dendrimers include polyvalency, self-assembly, chemical stability, electrostatic interactions, solubility and low cytotoxicity. Dendrimers are a good option in the medical and pharmaceutical industries due to their varied characteristics. Nanostar dendrimer is a collection of macromolecules that resemble photon funnels which is similar to artificial antennas and have a variety of applications.

The silicates are by far the largest, most significant, and complicated group of minerals. A silicate network is a ring of tetrahedrons with oxygen ions representing the corner vertices and the silicon ion representing the center vertex. A new network called an oxide network is created when all the silicon vertices in a silicate network are removed. Oxide networks are very important when studying silicate networks [2].

Carbon nanotubes, boron triangular nanotubes and boron α-nanotubes are the three most significant nanostructures. The first boron triangular nanotubes, made from a triangular sheet,

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were created in 2004 [3, 4]. Researchers [5–7] have created a particular boron sheet from a triangular sheet of boron in which one-ninth of the atoms will be absent. The term boron α-sheet refers to this unique boron sheet. Due to the remarkable properties like electronic structure, structural stability, transport properties, and work function, boron nanotubes are becoming increasingly interesting [8].

Polyomino graphs (finite 2-connected plane graph) have applications in modeling problems of surface chemistry and crystal physics [9, 10]. In a polyomino system, interior face is bordered by a regular square with a side length of one [11, 12]. A polyomino system, in which every square is connected to every other square by no more than two squares, is a polyomino chain.

Grünbaum introduced the concept of acyclic vertex coloring [13] and Jozef Fiamčik introduced the idea of acyclic edge coloring [14]. It is an NP-complete problem to calculate the number of cycles and the acyclic chromatic index for any graph [15, 16]. As a result, determining the acyclic chromatic index is challenging. For a given graph G and an integer k, A.V. Kostochka proved that determining whether the acyclic chromatic number of G is at most k, is an NP-complete problem [17].

The acyclic colorings of graphs have applications in various fields like multivariable calculus [18], optical networks [19], statistical mechanics [20], and so on. A Kekulé structure in a molecular graph is a perfect matching in the graph. The acyclic coloring of graphs enables categorization of Kekulé structures into equivalence classes of structures, where all of the structures in a class have the same resonance energy (measure of stability) [21]. Applications of the acyclic edge-colorings of graphs include enumeration of unsaturated isomers of a certain class of organic compounds [22].

Many significant results have been produced in acyclic coloring of graphs [23–25]. As far as we are aware, not much work has been done on finding the acyclic coloring of chemical structures except for the acyclic chromatic index of carbon nanosheets [26]. In this paper, utilizing the idea of vertex cut and matching, some chemical structures including nanostar dendrimers, silicate networks, oxide networks, boron nanosheets, and polyomino chains have been acyclically colored. We find the acyclic chromatic number $\chi_a(G)$ and acyclic chromatic index $\chi'_a(G)$ and prove that $\chi_a(G) \leq \chi'_a(G)$.

The rest of the paper is organized as follows. The definitions and other preliminaries are presented in Section 2. The key findings are laid up in Section 3. Finally, Section 4 concludes the paper with further research directions.

2 Basic concepts

A simple undirected graph G consists of the vertex set represented by V and the edge set represented by E. Thus, a graph $G = (V, E)$ is a mathematical representation of a network describing the relationship between its vertices and edges. Molecular graphs are frequently used to model molecules and molecular compounds. A molecular graph is a graph-theoretical depiction of the structural formula of a chemical compound, where the vertices represent the compound's atoms and the edges represent its chemical bonds. All the graphs considered in this paper are simple and finite. Let $deg(v)$ denote the *degree* of a vertex v, which is the number of edges incident to a vertex v of a graph G. Let $\Delta(G)$ denote the *maximum degree* of a graph G.

Matching theory is one of the most fundamental and significant theories in network flow theory and combinatorial theory. A *matching* M in G is a set of edges which are pairwise non-adjacent. A matching that cannot be extended by adding any more edges is called a maximal matching. If every vertex of G is covered by an edge of M, then the matching M is said to

be a *perfect matching*. In the chemical structure, an aromatic compound's Kekulé structure coincides with a perfect matching of its carbon skeleton, showing the locations of double bonds. If a perfect matching exists, a benzenoid system is Kekuléan.

A labeling $f\colon V(G) \to [k]$ is a *k-vertex coloring* of a graph G in which the labels are colors and a color class is a set of vertices with the same color. A k-vertex coloring is said to be *proper* if adjacent vertices have distinct colors. The *chromatic number* of a graph G is defined as the least number of colors required for a proper vertex coloring of G. A vertex coloring of a graph G is *acyclic* if it is a proper vertex coloring with no 2-colored (bichromatic) cycle in G [13]. Alternatively, the subgraph induced by the vertices of any two of the colors will not have any cycle in it. The *acyclic chromatic number* of G is the least number of colors in an acyclic coloring of G, which is denoted by $\chi_a(G)$.

A labeling $f\colon E(G) \to [k]$ is a *k-edge coloring* of a graph G. Here, the labels are colors, and a color class is a set of edges with the same color. The k edge-coloring of G is said to be *proper* if the adjacent edges have distinct colors. The *chromatic index* of a graph G is defined as the least number of colors required for a proper edge coloring of G. If there are no bichromatic cycles in a graph G, then the proper coloring of the edges of G is *acyclic* [14]. The least number of colors required to acyclically edge-color a graph G, denoted by $\chi'_a(G)$, is the *acyclic chromatic index* of G.

3 Main results

In this paper, we define the *f-vertex cut set* to find the acyclic chromatic number of nanostar dendrimer, oxide network, silicate network, boron nanosheet and polyomino chains.

Definition 3.1. Consider a graph G. A set $V \subset V(G)$ is called an f-vertex cut set (denoted by f_{vcs}) of G if the conditions listed below are satisfied.

(a) Each element in V is a cut vertex of G such that no two vertices in V share a common edge of G,

(b) $G \setminus V$ induces a forest in G.

3.1 Acyclic coloring of nanostar dendrimer

Nanostar dendrimers are one of the most fundamental nanobiotechnology objects having a wide range of applications in the medical field. It is denoted by D_n and has $(57(2^{n-1}) - 38)$ vertices and $(33(2^n) - 45)$ edges.

Theorem 3.2. $\chi_a(D_n) = 3$.

Proof. Consider the vertices v_i of degree 3 which are not part of a hexagon. Each of the adjacent vertices of v_i is an end vertex of the 6-cycle (hexagon) which forms the f-vertex cut set of D_n. The f-vertex cut set represents one color class (say 1) whose removal results in a forest. Each component of the forest is either a path, a tree or an isolated vertex.

Case 1: Path

A path is properly colored using two colors (say 2 and 3). The f-vertex cut set together with the path results in disjoint cycles of length 6. Since, the cycle is of even length, it can be properly colored using 3 colors.

Case 2: Tree

Two hexagons connected by an edge have their f-vertex cut set vertices to be the opposite end vertices, whose removal results in disjoint trees. The trees can be properly colored using

2 colors. The trees together with the vertices in the f-vertex cut set results in a 3-coloring ensuring the absence of bichromatic cycles.

Case 3: Isolated vertex

If one of the components of the forest is an isolated vertex, then it is always a vertex of degree 3. Each of its adjacent vertices belongs to the f-vertex cut set. Thus, the isolated vertex receives either color 2 or color 3. The isolated vertex together with the f-vertex cut set result in a tree. Hence, there exists no bichromatic cycles.

It can be seen that, in all of the above cases, only three colors have been used and there are no bichromatic cycles. Hence, for the nanostar dendrimer, the acyclic chromatic number is 3. See Figure 1(a). ■

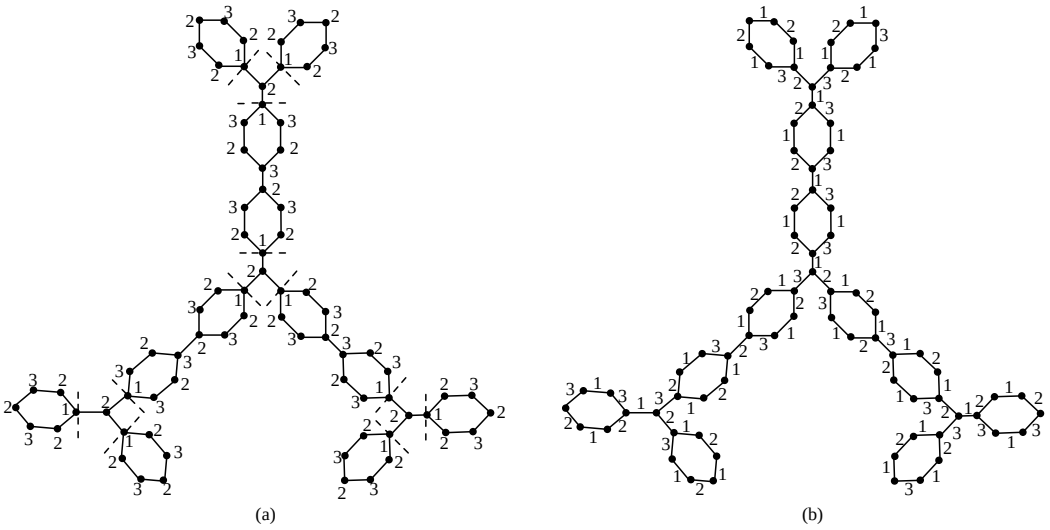

Figure 1: (a) Acyclic vertex coloring of nanostar dendrimer D_2. (b) Acyclic edge coloring of nanostar dendrimer D_2.

Theorem 3.3. $\chi'_a(D_n) = 3$.

Proof. Consider a maximal matching of D_n such that at least one of the edges, incident to a vertex with degree 3, is considered. The edges belonging to such a maximal matching form one color class (say 1). Consider the vertices of degree 3. One edge has been assigned color 1, by the previous argument. Hence, assign color 2 and 3 to the other two edges. Next, consider the hexagons with two edges colored 1. Then, the non-colored adjacent edges are assigned color 2 and 3, since they form a path. Consider the hexagons with three edges colored 1. Then, properly color at least one edge with color 2 and the remaining edges with color 3 so that there are no bichromatic cycles. For the remaining uncolored edges, assign color 2 or 3 such that a proper coloring of the edges is ensured. Thus, three colors are sufficient for the acyclic proper coloring. Hence, the ayclic chromatic index of D_n is 3. See Figure 1(b). ■

Remark 1. $\chi_a(D_n) = \chi'_a(D_n)$.

3.2 Acyclic coloring of oxide and silicate network

The silicate and oxide network are formed by the following procedure. Let $HC(n)$ be a hexagonal network of dimension n, where silicon ions are placed in its vertices. Then, place oxygen ions on the new vertices of $HC(n)$ obtained by subdividing each of its edges once. At each of the 2-degree silicon ions, introduce $6n$ new pendant edges. Then, on each of the pendant vertices, oxygen ions are placed. Each silicon ion associates with the three adjacent oxygen ions and they form a tetrahedron. This results in the silicate network $SL(n)$. In $SL(n)$, the parameter n represents the dimension. There are $15n^2 + 3n$ vertices and $36n^2$ edges in $SL(n)$. When all the silicon vertices are deleted from a silicate network, a new network called an oxide network is obtained. Let $OX(n)$ denote an n-dimensional oxide network. There are $9n^2 + 3n$ vertices and $18n^2$ edges in $OX(n)$.

Consider the following procedure for the formation of dominating oxide network and dominating silicate network. Consider a hexagonal network and place oxygen ions to its vertices obtained by subdividing each of its edges once. If the new vertices in a cell are separated by a distance of four units, connect them by an edge and add oxygen ions to the new edge crossings. Deleting the vertices and edges of the hexagonal network results in dominating oxide network $DOX(n)$. To get the dominating silicate network $DSL(n)$, place a silicon vertex to the centroid of each subgraph K_3 of dominating oxide network and connect it with other oxide vertex in the same K_3 [27].

Theorem 3.4. $\chi_a(OX(n)) = 3$.

Proof. The oxide network has $(4n + 1)$ levels. Every vertex in the odd levels represents the f-vertex cut set.The f-vertex cut set represents one color class (say 1) whose removal results in a forest. Each component of the forest is a path which can be properly colored using 2 colors (say 2 and 3). The union of f-vertex cut set together with the disjoint paths gives rise to cycles. To find the acyclic chromatic number and to ensure the absence of bichromatic cycles, it is enough to check for 3-cycles and 6-cycles.

Case 1: Cycles of length 3

Every 3-cycle can be acyclically colored using three colors. To check whether three colors are sufficient for all the cycles of length 3, consider the 3-cycle $C_1 = (v, v_1, v_2, v)$ adjacent to another 3-cycle $C_2 = (v, v_3, v_4, v)$, having a common vertex v. v either belongs to the f-vertex cut set or has colors 2 or 3. If $v \in f_{vcs}$, then the vertices v_1 and v_3 have color 2 whereas v_3 and v_4 have color 3. If v has color 2 or 3, then the other vertices have color 1 and 3 or the colors 1 and 2 respectively. This is because the 3-cycles are part of the f-vertex cut set and the disjoint paths. Hence, three colors are sufficient for a proper ayclic coloring.

Case 2: Cycles of length 6

Every edge of a 6-cycle is a common edge of the 3-cycles. Consider the labeling of the vertices of the 6-cycle as v_1, v_2, v_3, v_4, v_5 and v_6. Then, two of the opposite vertices belong to the f-vertex cut set. Let us call those vertices as v_3 and v_6. Removal of these vertices results in a path, which is the two opposite edges of the 6-cycle, namely (v_1, v_2) and (v_4, v_5). The vertices v_1 and v_2 have been assigned colors 2 and 3. Similarly, the vertices v_4 and v_5 have been assigned colors 2 and 3. Thus, every 6-cycle in the network has been assigned three colors.

It can be seen from case 1 and case 2 that, three colors are sufficient to properly color the entire network and there doesn't exist any bichromatic cycle. Hence, $\chi_a(OX(n)) = 3$. See Figure 2(a). ■

Theorem 3.5. $\chi'_a(OX(n)) = 4$.

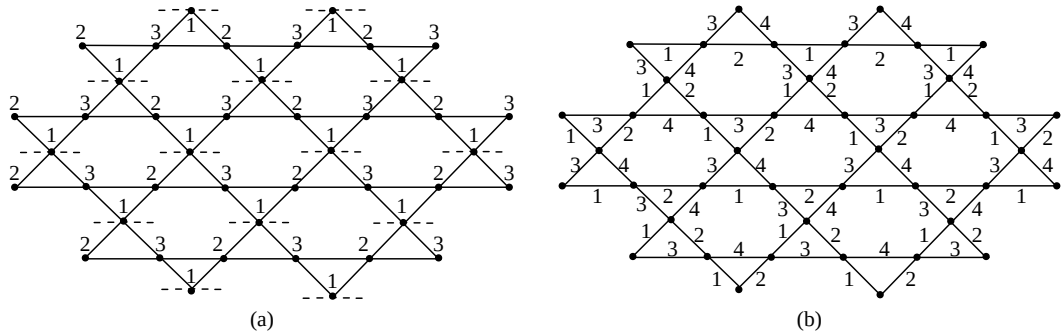

Figure 2: (a) Acyclic vertex coloring of oxide network $OX(2)$. (b) Acyclic edge coloring of oxide network $OX(2)$.

Proof. The oxide network $OX(n)$ can be given a proper and acyclic edge coloring using at least four colors, since $\Delta(OX(n)) = 4$. It has $(4n + 1)$ levels and every three levels in the network consists of a triangle and an inverted triangle joined by a common vertex. Denote the triangles (3-cycles) by (c, a, b, c) and (c, d, e, c), where c is the common vertex. The edges (a, c) and (c, e) are straight edges whereas the edges (a, b), (b, c), (c, d) and (d, e) are slanting edges. The straight edges and slanting edges form paths which can be colored using two colors each. Consider the following approach for a proper edge coloring of the oxide network:

For the levels 2, 6, ..., $4n - 2$, assign the colors 1 and 2 alternately to the straight edges. For the levels 4, 8, ..., $4n$, assign the colors 3 and 4 alternately to the straight edges. The slanting edges between the levels 1 and 3, 5 and 7, ..., $4n - 3$ and $4n - 1$ are assigned the colors 3 and 4 alternately. The slanting edges between the levels 3 and 5, 7 and 9, ..., $4n - 1$ and $4n + 1$ are assigned the colors 1 and 2 alternately.

Claim: Coloring by the above procedure is acyclic.

Every 3-cycle consists of a straight edge and two slanting edges. Hence, three colors are required for coloring the 3-cycles. Every edge of a 6-cycle consists of straight edges and slanting edges from six different cycles, thereby receiving four colors. Any cycle of length greater than six is either a part of the 3-cycle or a 6-cycle and hence must have at least three colors. Thus, the coloring is acyclic since there are no bichromatic cycles. Hence, $\chi'_a(OX(n)) = 4$. See Figure 2(b). ■

Corollary 3.6. *Each of the color class in the acyclic edge coloring of the oxide network OX(n) is a maximal matching.*

Remark 2. $\chi_a(OX(n)) < \chi'_a(OX(n))$.

Theorem 3.7. $\chi_a(SL(n)) = 4$.

Proof. By Theorem 3.4, a proper acyclic coloring of the oxide network requires at least three colors. The silicon vertex represents the internal vertex of the tetrahedron which is a complete graph on four vertices and can be properly colored using four colors. Therefore, the silicon vertex could be assigned the fourth color. Since the coloring of oxide network is proper and acyclic, it is ensured for the silicate network as well. Hence, $\chi_a(SL(n)) = 4$. See Figure 3(a). ■

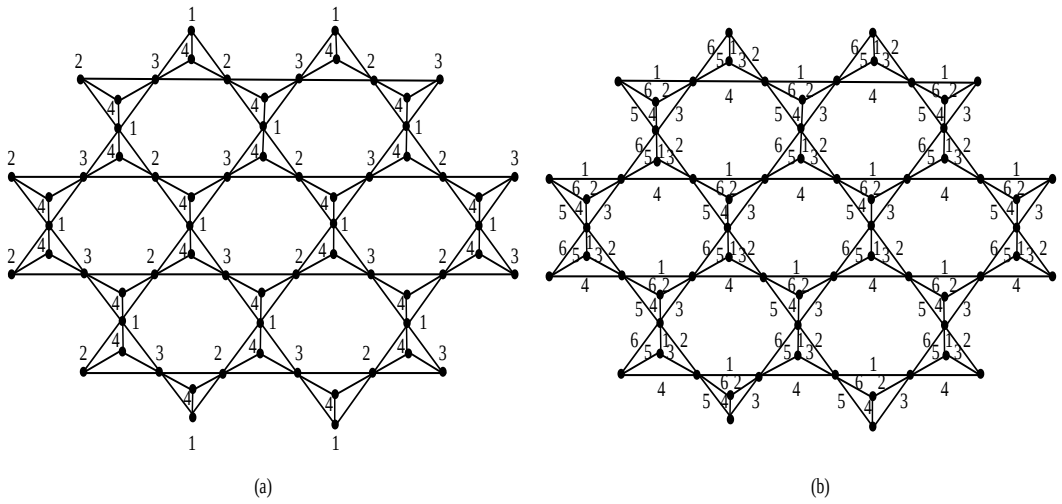

Figure 3: (a) Acyclic vertex coloring of silicate network $SL(2)$. (b) Acyclic edge coloring of silicate network $SL(2)$.

Theorem 3.8. $\chi'_a(SL(n)) = 6$.

Proof. The silicate network $SL(n)$ can be properly and acyclically edge colored using at least six colors, since $\Delta(SL(n)) = 6$. It consists of tetrahedrons and inverted tetrahedrons joined by a common vertex. Let T_1 be a tetrahedron consisting of the vertices v_1, v_2, v_3 and v_4. Let T_2 be an inverted tetrahedron on the left of T_1 consisting of the vertices v_4, v_5, v_6 and v_7. Here, v_4 is common to both the tetrahedrons. Also, assume that v_1 and v_7 are the central vertices of T_1 and T_2 respectively. Further, let v_3 be the top vertex of T_1 and v_5 be the bottom vertex of T_2. The colors 1, 2, 3, 4, 5 and 6 are assigned to the edges (v_4, v_6), (v_4, v_7), (v_4, v_5), (v_4, v_2), (v_4, v_1) and (v_4, v_3) respectively. Then, for the remaining edges, assign the colors 1, 2 and 3 to the edges opposite to the edges colored 4, 5 and 6 respectively and vice versa. This procedure is repeated for all the tetrahedrons in the network. The coloring is proper, since every edge incident on a common vertex receives different colors. Further, every edge in a tetrahedron gets six different colors. Hence, every 3-cycle gets three distinct colors. Therefore, the coloring is acyclic, since there are no bichromatic cycles. Also, six colors are enough for the proper acyclic coloring of the silicate network. Hence, $\chi'_a(SL(n)) = 6$. See Figure 3(b). ■

Corollary 3.9. *Each color class in the acyclic edge coloring of the silicate network SL(n) is a maximal matching.*

Remark 3. $\chi_a(SL(n)) < \chi'_a(SL(n))$.

Remark 4. The results obtained for the oxide and silicate network are true for the dominating oxide and dominating silicate network.

3.3 Acyclic coloring of boron nanosheet

A boron triangular sheet is a chemical graph obtained from a hexagonal sheet by including one additional atom to the center of each hexagon. By creating an assortment of triangles and hexagons, a special boron sheet has been designed from the original boron triangular sheet known as the boron α-sheet which lacks one-ninth of the atoms [6, 7]. We denote the boron triangular sheet by BS and the boron α-sheet by BS_α.

Theorem 3.10. $\chi_a(BS) = 4$.

Proof. Consider the oxide network after the removal of the vertices protruding from the hexagons on the outer boundary. Then, the boron triangular sheet, with the deletion of center atom in every hexagon, resembles the oxide network. By Theorem 3.4, the oxide network has an acyclic chromatic number 3. Further, the center atom could be assigned a new color say 4. This coloring is proper as all adjacent vertices get distinct colors. Further, there are no bichromatic cycles. This is because the center atom, which is adjacent to all the vertices in a hexagon has been assigned a new color. The coloring of the oxide network is acyclic, thereby ruling out the presence of bichromatic cycles. Hence, $\chi_a(BS) = 4$. See Figure 4(a). ■

Corollary 3.11. $\chi_a(BS_\alpha) = 4$.

Proof. By the definition of boron α-sheet, since some of the atoms are missing from the original boron sheet, the acyclic vertex coloring remains the same. Therefore, $\chi_a(BS_\alpha) = 4$. ■

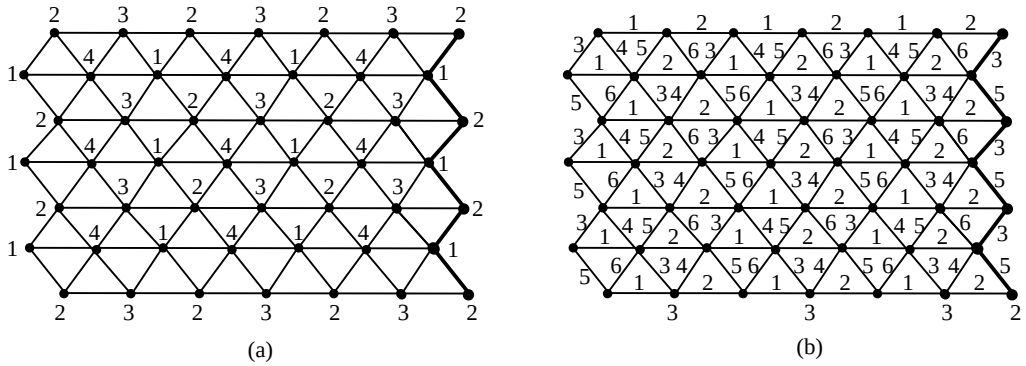

Figure 4: (a) Acyclic vertex coloring of boron network BS. (b) Acyclic edge coloring of boron network BS.

Theorem 3.12. $\chi'_a(BS) = 6$.

Proof. The boron triangular sheet can be properly and acyclically edge colored using at least six colors, since $\Delta(BS) = 6$. Consider a perfect matching consisting of alternate edges in every row. It forms one color class (say 1). Since every row is a path, which could be acyclically colored using two colors, the remaining edges in the row are colored using color 2. Consider a hexagon with the central atom. The edges between the first two rows could be assigned four distinct colors say 3, 4, 5 and 6 in order and the edges between the second and third rows could

be assigned the colors 5, 6, 3 and 4 in order. This procedure is repeated for the remaining edges in the nanosheet. The coloring is proper, since every edge incident on a common vertex receives different colors. Further, every edge connecting the vertices of a hexagon to the central atom gets six different colors. Hence, every 3-cycle gets three distinct colors. Therefore, the coloring is acyclic due to the absence of bichromatic cycles. Also, six colors are enough for the proper acyclic coloring. Hence, $\chi'_a(BS) = 6$. See Figure 4(b). ■

Corollary 3.13. $\chi'_a(BS_\alpha) = 6$.

Proof. By the definition of boron α-sheet, since some of the atoms are missing from the original boron sheet, the acyclic edge coloring remains the same. Therefore, $\chi'_a(BS_\alpha) = 6$. ■

Remark 5. $\chi_a(BS) < \chi'_a(BS)$ and $\chi_a(BS_\alpha) < \chi'_a(BS_\alpha)$.

3.4 Acyclic coloring of polyomino chain system

A k-polyomino system has each of its interior face being surrounded by a regular $4k$-cycle of length one [12]. Terminal (respectively non-terminal) refers to a square that is adjacent to just one (respectively two) additional square(s). A non-terminal square with a degree 2 vertex is called a kink. A segment is the longest possible linear chain in a polyomino chain which includes any terminal squares and/or kinks at its ends. In particular, the zig-zag chain Z_n and the linear chain L_n with exactly one segment are polyomino chains of length n and 2 respectively. The polyomino chain system is denoted by P_n^k with two defining parameters k and n , where k is the sum of the number of kinks and number of terminals in a unit of any particular polyomino chain and n is the defining parameter (dimension) of the chain. P_n^k has $3kn + 1$ edges.

Theorem 3.14. $\chi_a(P_n^k) = 3$.

Proof. Consider any set of vertices whose removal results in a forest as a f-vertex cut set f_{vcs} in the polyomino chain system. Deleting all the vertices from f_{vcs} leaves the graph with connected components where each component consists of a path or a tree which is acyclic. For an acyclic graph, the acyclic chromatic number corresponds to the chromatic number of the graph which is two. One color could be assigned to all the vertices in f_{vcs}. Hence, three colors are required for the acyclic coloring of polyomino chains. The coloring is proper since adjacent vertices get distinct colors. Further, any two cycles are connected by means of a common edge. Hence, there are no bichromatic cycles as every cycle gets three distinct colors. Thus, the acyclic chromatic number of polyomino chain system is three. See Figure 5(a). ■

Theorem 3.15. $\chi'_a(P_n^k) = \Delta$.

Proof. Consider a perfect matching of the graph. The edges of this perfect matching form one color class. Deletion of these edges results in a forest which could be colored with a maximum of $\Delta - 1$ colors. Further, any two cycles are connected by means of a common edge. Hence, there are no bichromatic cycles. Thus, Δ colors are required for the acyclic coloring of polyomino chain system. See Figure 5(b). ■

Remark 6. $\chi_a(P_n^k) \leq \chi'_a(P_n^k)$, since $\Delta(P_n^k)$ is either 3 or 4.

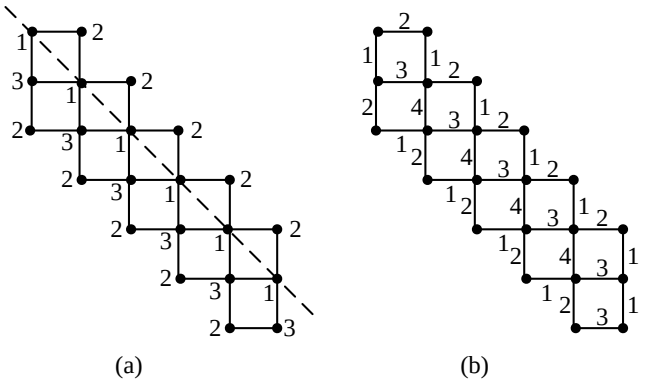

Figure 5: (a) Acyclic vertex coloring of polyomino chain P_5^2. (b) Acyclic edge coloring of polyomino chain P_5^2.

4 Concluding remarks

In this paper, we have considered the concept of vertex cut and matching to find the acyclic coloring parameters for certain chemical structures like nanostar dendrimer, oxide network, silicate network, boron nanosheets, and polyomino chains. Also, we have proved that $\chi_a(G) \leq \chi'_a(G)$ for all the networks under consideration. As a further research direction, chemical structure of drugs will be explored along with their properties and the application of acyclic coloring parameters to pharmaceuticals will be investigated.

Author Contributions: A. Berin Greeni and V. Vinitha Navis conceived of the presented idea. V. Vinitha Navis developed the theory and performed the computations. A. Berin Greeni verified the analytical methods and encouraged V. Vinitha Navis to investigate the acyclic coloring parameters and supervised the findings of this work. All authors discussed the results and contributed to the final manuscript.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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