A New Approach to Compute Acyclic Chromatic Index of Certain Chemical Structures

I. RAJASINGH, R. S. RAJAN AND D. PAUL

School of Advanced Sciences, VIT University, Chennai-600127, India

Correspondence should be addressed to paul.d.joe@gmail.com

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ABSTRACT An acyclic edge coloring of a graph is a proper edge coloring such that there are no bichromatic cycles. The acyclic chromatic index of a graph G denoted by $\chi_a^{'}(G)$ is the minimum number k such that there is an acyclic edge coloring using k colors. The maximum degree in G denoted by $\Delta(G)$, is the lower bound for $\chi_a^{'}(G)$. P–cuts introduced in this paper acts as a powerful tool to prove that this bound is sharp for certain chemical structures.

KEYWORDS Acyclic edge–coloring · acyclic chromatic index · maximum degree · certain chemical structures.

1. INTRODUCTION

A molecular graph is a collection of vertices representing the atoms in the molecule and a set of edges representing the covalent bonds. Graph representation of molecular structures is widely used in computational chemistry [1]. A coloring of the edges of a graph is proper if no pair of incident edges receive the same color. The edge-colorings of graphs are shown to be useful in multiple quantum Nuclear Magnetic Resonance(NMR) from which one would obtain various types of dipolar couplings present in a molecule. The question then is in how many different ways could one assemble the dipolar couplings. Each such way corresponds to a possible structure of the unknown compound. The edge-colorings of graphs are shown to enumerate unique dipolar interactions amoung a given set of nuclei thereby providing a technique for structure elucidation from NMR [2, 3].

A proper coloring of the edges of a graph is acyclic if there is no two-colored (bichromatic) cycle in that graph. In other words, the subgraph induced by the union of any two color classes is a forest. The minimum number of colors required to edge-color a graph acyclically is termed the acyclic chromatic index. The notion of acyclic coloring was introduced by Grunbaum [4]. Determining acyclic chromatic index for an arbitrary graph is an NP-complete problem [5]. The problem of determining the number of cycles in a graph is NP-complete [6]. Therfore computing acyclic chromatic index even for very special classes of graphs is challenging. The acyclic edge-colorings of graphs are also shown to have applications in the enumeration of unsaturated isomers of a class of organic compounds [7]. They also have applications in statistical mechanics in enumerating the number of statistical mechanical diagrams [8]. Further the acyclic edge-coloring of graphs enables classification of kekule structures into equivalence classes of structures such that all structures in a class have the same resonance energy [10, 9].

The results obtained so far use only probablistic methods of proof [11]. In this paper we compute the exact acyclic edge-chromatic index of certain chemical structures by introducing *P*–cuts.

2. ACYCLIC CHROMATIC INDEX USING P-CUTS

We give the basic definitions and preliminaries which are required for the remaining study. A graph G is an ordered triple $(V(G), E(G), \varphi(G))$ consisting of a non-empty set $V(G)$ of vertices, a set $E(G)$ disjoint from $V(G)$ of edges and an incident function $\varphi(G)$, that associates with each edge of G an unordered pair of (not necessarily distinct) vertices of G. The degree of a vertex of a graph G is the number of edges incident to the vertex, with loops counted twice. The degree of a vertex v is denoted as $\deg(v)$. The maximum degree of a graph G is denoted by $\Delta(G)$.

Definition 2.1 [12] *A proper edge-coloring of a graph G is an assignment of "colors" to the edges of G such that no two adjacent edges receive the same color. The minimum number of colors required to edge-color a graph G is termed as chromatic index of G and is denoted by $\chi'(G)$.*

Definition 2.2 [13, 14] *A proper edge-coloring of a graph G is acyclic if there is no two-colored (bichromatic) cycle in G. The minimum number of colors required to edge-color a graph G acyclically is termed as acyclic chromatic index of G and is denoted by $\chi_a^{'}(G)$.*

Definition 2.3 [15] *The girth of a graph G is the length of a shortest cycle contained in G.*

Definition 2.4 [16] *An edge-cut of a graph G is a set of edges in G whose removal produces a subgraph with more components than the original graph G.*

Lemma 2.5 [17] *Let* G *be any planar graph, then* $\chi_a^{'}(G) \geq \chi'(G) \geq \Delta(G)$.

We inroduce a technique to compute acyclic chromatic index $\chi_a^{'}(G)$ in planar graphs. We define P-cuts in planar graphs to obtain lower bound on $\chi_a^{'}(G)$ and prove that the bound is sharp for certain chemical structures.

Definition 2.6 *Let* G *be a planar graph and* $S = \{S_1, S_2, \ldots S_k\}$ *be a collection of subsets of* $E(G)$. S *is called a* P*-cut if it satisfies the following conditions:*

1. Each S_i is an edge-cut of G such that $|S_i| \geq 3$ and no two edges in S_i share a common vertex of G, $1 \leq i \leq k$.
2. No edge in S_i is adjacent to any edge in S_j, $i \neq j, 1 \leq i$, $j \leq k$.
3. $G \setminus \{\bigcup_{i=1}^{k} S_i\}$ induces a partition $V_1, V_2, .., V_{k+1}$ of $V(G)$, each inducing a path in G.

Theorem 2.7 *Let* G *be a planar graph. If* G *has a* P*-cut, then* $\Delta(G) = 3$.

Proof. Removal of set of edges in G disconnects the graph into $k+1$ disjoint paths. The maximum degree of path is 2. Every cycle in G passes through at least two edges of some S_i. Therefore the maximum degree of G is increased by one. Hence $\Delta(G) = 3$.

Theorem 2.8 *Let* G *be a planar graph of girth* $\geq$ 4. If G has a P-cut, then $\chi_a^{'}(G) = 3$.

Proof. For every pair of edges (u, x) and (v, y) in S_i

Case (i): $d(u,v) = d(x, y)$ and girth $\geq$ 4.

Color the edges in $\cup_{i=1}^{k} s_i$ with color c_1. Any path has an acyclic chromatic number 2 and hence it can be colored with 2 colors. Color the paths P^i induced by $G \setminus \{\cup_{i=1}^{k} s_i\}$ using colors c_2 and c_3. Every cycle in G passes through at least two edges of some S_i. Since the length of the paths are equal, any cycle formed will be colored with three colors.

Case (ii): $d(u,v) \neq d(x, y)$ and girth $\geq$ 5.

Color the edges in $\cup_{i=1}^{k} s_i$ with color c_1. Any path has an acyclic chromatic number 2 and hence it can be colored with 2 colors. Color the paths P^i induced by $G \setminus \{\bigcup_{i=1}^{k} S_i\}$ using colors c_2 and c_3. Every cycle in G passes through at least two edges of some S_i. Since there is no 4-cycle in G, any cycle formed will be colored with three colors.

Case (iii): $d(u,v) \neq d(x,y)$ and girth = 4.

Color the path P^i induced by $G \setminus \{\bigcup_{i=1}^{k} S_i\}$ except for the edges in the four cycle by c_1 and c_2. Color the edges in S_i by c_2 and c_3 or c_3 and c_1 such that every cycle of girth ≥ 5 has two different colors in S_i. Color the four cycle in such a way that if two edges in S_i has same color then color the remaining two edges by other two colors and if two edges in S_i has different color then color the remaining two edges by remaining one color. Every four cycle in G is colored with three colors. Every cycle in G passes through at least two edges of some S_i and therefore any cycle of girth ≥ 5 will be colored with three colors. Hence any cycle formed will be colored with three colors.

3. NANOSHEETS WITH ACYCLIC CHROMATIC INDEX 3

Carbon nanosheets are a new kind of two-dimensional polymeric material that is fabricated by cross-linking aromatic self-assembled monolayers with electrons. Due to their uniform thickness of only about one nanometer, as well as their high chemical, mechanical, and thermal stability, such materials are of high interest for a wide variety of applications[18]. As the nanosheet is stable under an electron beam, patterns can also be written by electron beam induced deposition (EBID). Because of their stability and flexibility, carbon nanosheets will likely find a multitude of applications, including potential use as sensors, filtration membranes, sample supports, and even conductive coatings [19].

3.1 $C_4C_8(R)[2m,2n]$ Nanosheet

A $C_4C_8(R)[2m,2n]$ nanosheet is a trivalent decoration made by alternating squares C_4 and octagons C_8 and it is a bi-regular graph with m number of rows and n number of columns. The $C_4C_8(S)[2m,2n]$ nanosheet has $4(m+1)(n+1)$ vertices [1, 20].

Theorem 3.1 *Let G be a $C_4C_8(R)[2m,2n]$ nanosheet. Then* $\chi_a^{'}(G) = 3$.

Proof. Let G be a $C_4C_8(R)[2m,2n]$ nanosheet and $S = \{S_1, S_2, \ldots S_{2n}\}$ be a set of P-cuts, such that removal of edges in P-cuts disconnects the graph into disjoint paths. See Figure

1. By Theorem 2.8, $\chi'_a(G) = 3$.

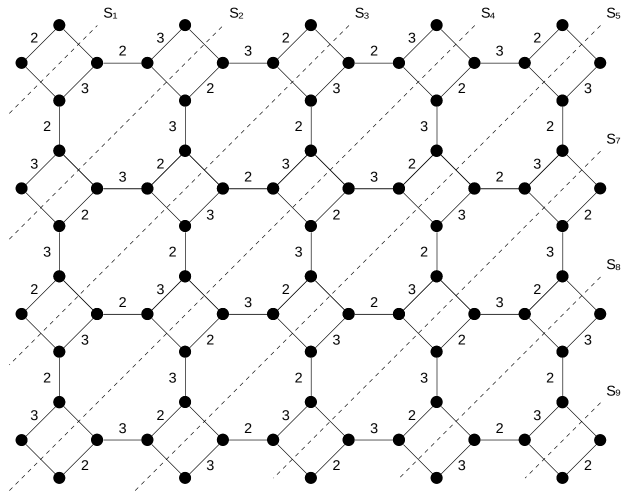

Figure 1. Acyclic edge-coloring of $C_4C_8(R)[6,8]$ nanosheet.

3.2 $C_4C_8(S)[2m,2n]$ Nanosheet

A $C_4C_8(S)[2m,2n]$ nanosheet is a trivalent decoration made by alternating squares C_4 and octagons C_8 and is a bi-regular graph with m number of rows and n number of columns. It is a bipartite graph. The $C_4C_8(S)[2m,2n]$ nanosheet has $8mn$ vertices [21].

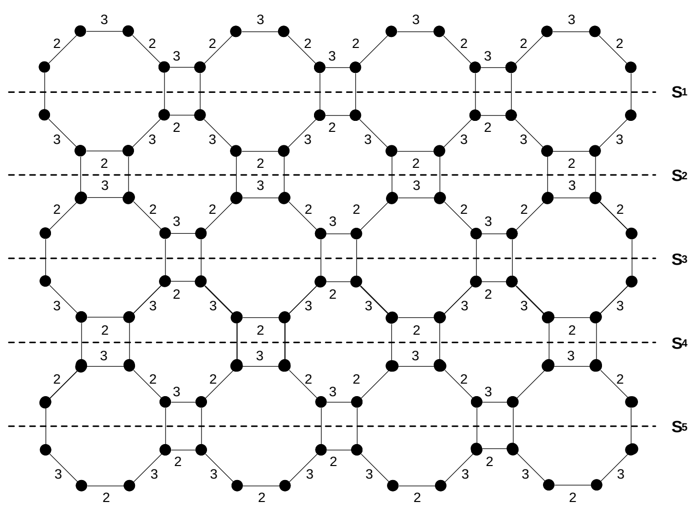

Figure 2. Acyclic edge-coloring of $C_4C_8(S)[6,8]$ nanosheet.

Theorem 3.2 *Let G be a $C_4C_8(S)[2m,2n]$ nanosheet. Then* $\chi_a^{'}(G) = 3$.

Proof. Let G be a $C_4C_8(S)[2m,2n]$ nanosheet and $S = \{S_1, S_2,..S_{2m-1}\}$ be a set of P-cuts, such that removal of edges in P-cuts disconnects the graph into disjoint paths. See Figure 2. By Theorem 2.8, $\chi_a^{'}(G) = 3$.

3.3 $C_6[m,n]$ Nanosheet

A $C_6[m,n]$ nanosheet is a trivalent decoration made by haxagon C_6 and it is a bi-regular graph with m number of rows and n number of columns. A nanosheet with wrap-around edges is called a nanotube. A $C_6[m,n]$ nanotube is called as Peri-condensed Benzenoids graph. The $C_6[m,n]$ nanosheet has $4(n+2)m$ vertices [1, 22].

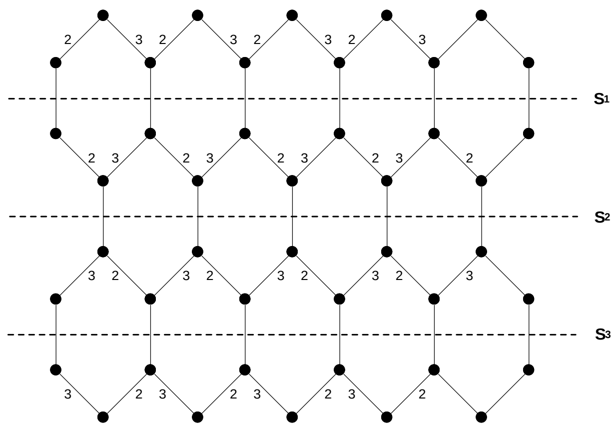

Figure 3. Acyclic edge-coloring of $C_6[3,5]$ nanosheet.

Theorem 3.3 *Let G be a $C_6[m,n]$ nanosheet. Then* $\chi_a^{'}(G) = 3$.

Proof. Let G be a $C_6[m,n]$ nanosheet and $S = \{S_1, S_2,..S_m\}$ be a set of P-cuts, such that removal of edges in P-cuts disconnects the graph into disjoint paths. See Figure 3. By Theorem 2.8, $\chi_a^{'}(G) = 3$.

3.4 $C_5C_6C_7[m,n]$ Nanosheet

A $C_5C_6C_7[m,n]$ nanosheet is a trivalent decoration made by alternating pentagon C_5, hexagon C_6 and septagon C_7 and is a bi-regular graph with m number of rows and n number of columns. The $C_5C_6C_7[m,n]$ nanosheet has $16mn+2m$ vertices [23].

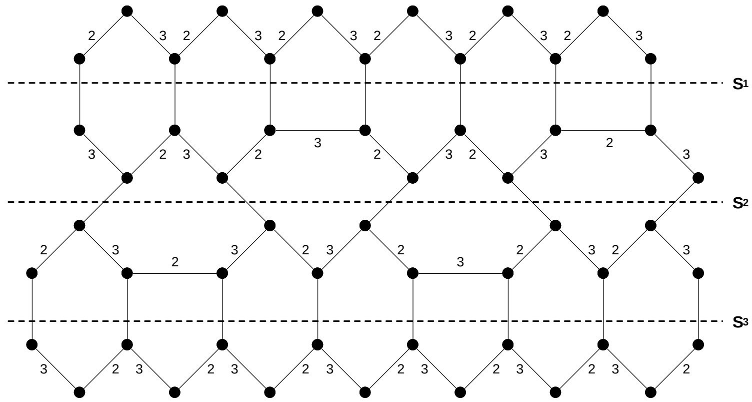

Figure 4. Acyclic edge-coloring of $C_5C_6C_7[3,6]$ nanosheet.

Theorem 3.4 *Let G be a $C_5C_6C_7[m,n]$ nanosheet. Then* $\chi_a^{'}(G)=3$.

Proof. Let G be a $C_5C_6C_7$ nanosheet and $S=\{S_1,S_2,..S_m\}$ be a set of P-cuts, such that removal of edges in P-cuts disconnects the graph into disjoint paths. See figure 4. By Theorem 2.8, $\chi_a^{'}(G)=3$.

3.5 $C_5C_7[m,n]$ Nanosheet

A $C_5C_7[m,n]$ nanosheet is a trivalent decoration made by alternating hexagons C_5 and septagons C_7 and is a bi-regular graph with m number of rows and n number of columns. The $C_5C_7[m,n]$ nanosheet has $8mn+m$ vertices [23].

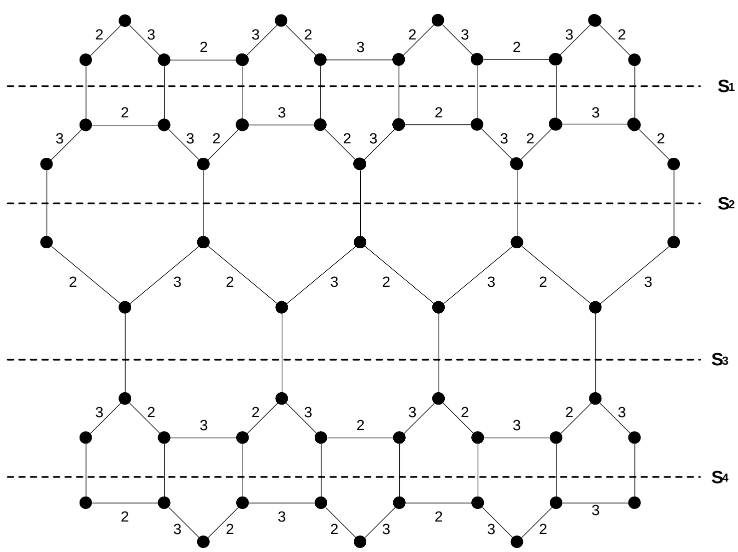

Figure 5. Acyclic edge-coloring of $C_5C_7[4,7]$ nanosheet.

Theorem 3.5 *Let G be a $C_5C_7[m,n]$ nanosheet. Then* $\chi'_a(G) = 3$.

Proof. Let G be a $C_5C_7[m,n]$ nanosheet and $S = \{S_1, S_2, ..S_m\}$ be a set of P-cuts, such that removal of edges in P-cuts disconnects the graph into disjoint paths. See Figure 5. By Theorem 2.8, $\chi'_a(G) = 3$.

3.6 $C_4C_6C_8[2m,2n]$ Nanosheet

A $C_4C_6C_8[2m,2n]$ nanosheet is a trivalent decoration made by alternating squares C_4, hexagons C_6 and octagons C_8 and is a bi-regular graph with m number of hexagons in each row and n number of hexagons in each column. The $C_4C_6C_8[2m,2n]$ nanosheet has $6mn$ vertices.

Theorem 3.6 *Let G be a $C_4C_6C_8[2m,2n]$ nanosheet. Then* $\chi'_a(G) = 3$.

Proof. Let G be a $C_4C_6C_8[2m,2n]$ nanosheet and $S = \{S_1, S_2, ..S_m\}$ be a set of P-cuts, such that removal of edges in P-cuts disconnects the graph into disjoint paths. See Figure 6. By Theorem 2.8, $\chi'_a(G) = 3$.

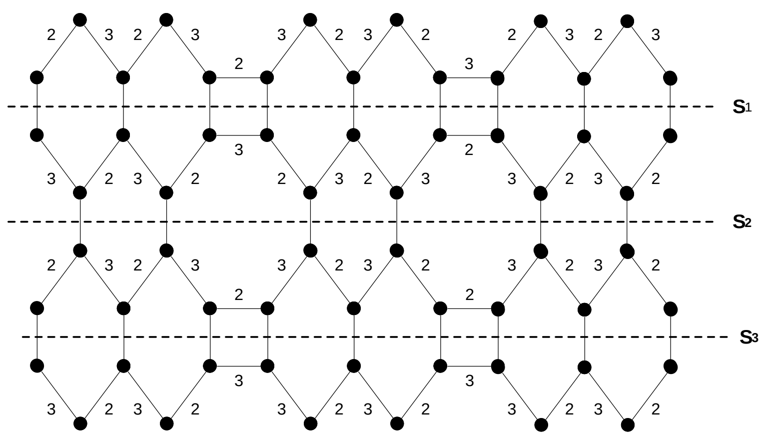

Figure 6. Acyclic edge-coloring of $C_4C_6C_8[4,8]$ nanosheet.

3.7 H-Naphtalenic [$2m,2n$] Nanosheet

A H-Naphtalenic [$2m,2n$] nanosheet is a trivalent decoration made by alternating squares C_4,pair of hexagons C_6 and octagons C_8 and it is a bi-regular graph with m number of rows and n number of columns. The H-Naphtalenic [$2m,2n$] nanosheet has $10mn$

vertices [1, 24].

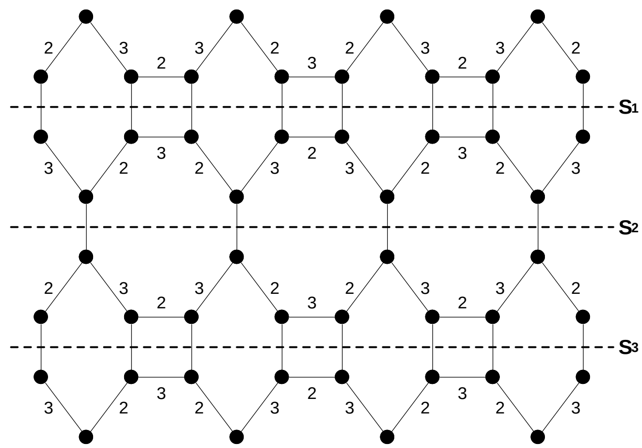

Figure 7. Acyclic edge-coloring of H -Naphtalenic [4,6] nanosheet.

Theorem 3.7 *Let G be a H -Naphtalenic* $[2m,2n]$ *nanosheet. Then* $\chi_a^{'}(G) = 3$.

Proof. Let G be a H -Naphtalenic $[2m,2n]$ nanosheet and $S = \{S_1, S_2,..S_{2m-1}\}$ be a set of P -cuts, such that removal of edges in P -cuts disconnects the graph into disjoint paths. See Figure 7. By Theorem 2.8, $\chi_a^{'}(G) = 3$.

4. Conclusion

In this paper we have proved that $\chi_a^{'}(G) = \Delta(G)$ for certain nanosheets. The problem of acyclic edge-coloring of certain chemical structures with chromatic number $\Delta(G)+1$ is under investigation.

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