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Strong chromatic index of certain nanosheets

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Abstract. Strong edge-coloring of a graph is a proper edge coloring such that every edge of a path of length 3 uses three different colors. The strong chromatic index of a graph is the minimum number k such that there is a strong edge-coloring using k colors and is denoted by $\chi'_s(G)$. We give efficient algorithms for strong edge-coloring of certain nanosheets using optimum number of colors.

Keywords: strong edge-coloring, strong chromatic index, nanosheets
Mathematics Subject Classification (2010): 05C15.

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. A coloring of the edges of a simple graph is proper if no pair of incident edges receives the same color. The edge-colorings of graphs are shown to be useful in multiple quantum Nuclear Magnetic Resonance (NMR) from which one could obtain various types of dipolar couplings present in a molecule. These dipolar couplings can be assembled in different ways. Each such way corresponds to a possible structure of the unknown compound. The edge-colorings of graphs are shown to enumerate unique dipolar interactions among a given set of nuclei, thereby providing a technique for structure elucidation from NMR [3].

A proper coloring C of the edges of a graph G is strong, if the edges of every path of length 3 uses three different colors. Strong edge-coloring is also known as distance 2 edge

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coloring. A strong edge coloring of a graph is equivalent to a partition of the set of edges into a collection of induced matchings. The minimum number of colors required to edge color a graph G strongly is termed as strong chromatic index of G and is denoted by $\chi'_s(G)$. Strong edge-coloring was introduced by Fouquet and Jolivet in 1983 [9]. Strong edge coloring is an NP-complete problem [17]. The strong edge-colorings of graphs are also shown to have applications in the enumeration of unsaturated isomers of a class of organic compounds [2,3]. They also have applications in statistical mechanics in enumerating the number of statistical mechanical diagrams [20]. The study of kekule structures of chemical compounds have many hidden treasures [21] and have for a long time been the focus of interest of scholars working on the theory of benzenoid molecules [13]. A vast amount of theoretical work also has been done on kekule structures [11,14]. Further the strong 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 [12,18].

2 Preliminaries

Definition 1. [4,6] A proper edge coloring of a graph G is an assignment of "colors" to the edges of the graph G so that no two adjacent edges have the same color. The minimum number of colors required to color a graph G is known as chromatic index of graph G and is denoted by $\chi'(G)$.

Definition 2. [8] A proper edge-coloring of a graph G is strong if every path of length 3 receives three different colors. The minimum number of colors required to edge-color a graph G strongly is termed as strong chromatic index of G and is denoted by $\chi'_s(G)$.

Definition 3. [6] For a graph G, let $V(G)$ and $E(G)$ denote the vertex set and edge set of G respectively. We say that H is a subgraph of G if $V(H) \subseteq V(G)$ and $E(H) \subseteq E(G)$.

Definition 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 2.1. *Let H be a graph obtained from the cycle C_4, on 4 vertices, by adding a pendent edge at two adjacent vertices of C_4. See Figure* 1. *Then $\chi'_s(H) = 6$.*

Proof. By definition the edges of C_4 with 4 distinct colors. Paths of length 3 in H which include a pendent edge as one of the edges include every edge of C_4 in some path. Hence a new color has to be assigned to each of the pendent edges. Therefore $\chi'_s(H) = 6$. □

Lemma 2.2. [7] *If H is a subgraph of G, then $\chi'_s(G) \geq \chi'_s(H)$.*

3 Nanosheets with strong chromatic index 6

Carbon nanosheets are mechanically stable two-dimensional materials with a thickness of 1 nm and well defined physical and chemical properties. They are made by radiation

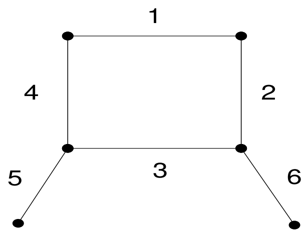

Figure 1. The graph H.

induced cross-linking of aromatic self-assembled monolayers. 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, semiconductors and even conductive coatings [22].

Carbon nanosheets are predicted to have many unique properties, such as magnetic moments 1000 times larger than previously expected for certain specific radii, or may be used as a black body whose emissivity or absorbance is almost one [15].

Edges of nanosheet drawn horizontally are called horizontal edges, perpendicular to the horizontal edges are called vertical edges, those edges that make an acute angle with the horizontal edges are called acute edges and those edges that make an obtuse angle with the horizontal edges are called obtuse edges.

3.1 $C_4C_8(S)[2m;2n]$ nanosheet

A $C_4C_8(S)[2m;2n]$ nanosheet is a trivalent decoration made by alternating squares C_4 and octagons C_8 [10]. It is a bi-regular graph with m number of rows and n number of columns, each column comprising of octagons C_8 viewed vertically and each row comprising of octagons C_8 viewed horizontally. It is a bipartite graph. The $C_4C_8(S)[2m;2n]$ nanosheet has $8mn$ vertices. See Figure 2.

A channel of C_8's and C_4's alternatively arranged horizontally beginning and ending with C_8 is termed a *row*. Similarly a channel of C_8's and C_4's alternatively arranged vertically is termed a *column* of $C_4C_8(S)[2m;2n]$. The following result is an easy consequence of Lemma 2.1 and Lemma 2. 2.

Lemma 3.1. *The strong chromatic index of $C_4C_8(S)[2m;2n]$ is at least 6.*

The algorithm 3.2 given below shows that $\chi'_s(C_4C_8(S)[2m;2n]) = 6$.

Let a, o, v_4, v_8, h_4, h_8 denote an acute edge, an obtuse edge, a vertical edge of C_4, a vertical edge of C_8, a horizontal edge of C_4 and a horizontal edge of C_8 respectively. Acute, obtuse, vertical and horizontal edge-cuts are shown in Figure 2.

3.2 Algorithm for $C_4C_8(S)[2m;2n]$ nanosheet

Input: $C_4C_8(S)[2m;2n]$ nanosheet
Algorithm:

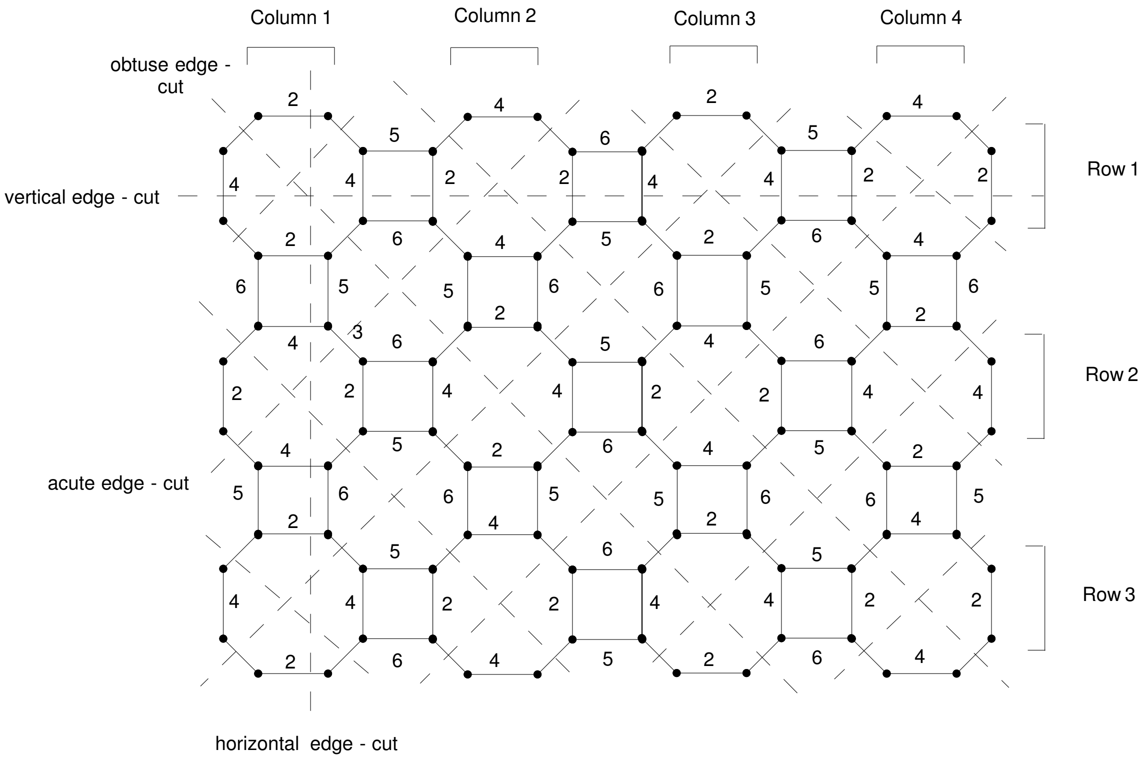

Figure 2. Strong edge-coloring of $C_4C_8(S)[6,8]$ nanosheet.

Step 1: Color obtuse edge-cuts as 1.
Step 2: Color acute edge-cuts as 3.
Step 3: Color v_8 - edge-cuts of Row i i odd, sequentially as 4,4, 2,2, 4,4. . . .
Step 4: Color v_8 - edge-cuts of Row i, i even, sequentially as 2,2, 4,4, 2,2. . . .
Step 5: Color h_8 - edge-cuts of Column i, i odd, sequentially as 2,2, 4,4, 2,2. . . .
Step 6: Color h_8 - edge-cuts of Column i, i even, sequentially as 4,4, 2,2, 4,4. . . .
Step 7: Color h_4 - edge-cuts of Column i, i odd, sequentially as 5,6, 6,5, 5,6. . . .
Step 8: Color h_4 - edge-cuts of Column i, i even, sequentially as 6,5, 5,6, 6,5. . . .
Step 9: Color v_4 - edge-cuts of Row i, i odd, sequentially as 6,5, 5,6, 6,5. . . .
Step 10: Color v_4 - edge-cuts of Row i, i even, sequentially as 5,6, 6,5, 5,6. . . . See Figure 2.
Output:$\chi'_s(C_4C_8(S)[2m;2n]) = 6$.
Proof of correctness: Let G be $(C_4C_8(S)[2m;2n]$ nanosheet. Paths of length 3 in G are of the following category.
1. The 3 edges are distinct members of the set $X = \{a, o, v_4, v_8, h_4, h_8\}$.
2. One edge is h_4 and the other two are v_4.
3. One edge is v_4 and the other two are h_4.
In all three cases the edges receive distinct colors.

The following theorem is an easy consequence of Lemma 3.1 and the Algorithm 3.2.

Theorem 3.2. *Let G be a* $C_4C_8(S)[2m;2n]$ *nanosheet. Then* $\chi_s'(G) = 6$*.*

4 $C_4C_8(R)[2m;2n]$ 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 $C_4C_8(R)[2m;2n]$ nanosheet has $4(m+1)(n+1)$ vertices [1]. A channel of C_4 and K_2 arranged horizontally beginning and ending with C_4 is termed a row. Similarly a channel of C_4 and K_2 arranged vertically is termed a column of $C_4C_8(R)[2m;2n]$. Consider a C_4 in $C_4C_8(R)[2m;2n]$ as shown in Figure 3. Name the edges as TL, TR, BL and BR representing Top Left, Top Right, Bottom Left and Bottom Right. The following algorithm always labels the obtuse edges in the order TL and BR, the acute edges in the order TR and BL respectively.

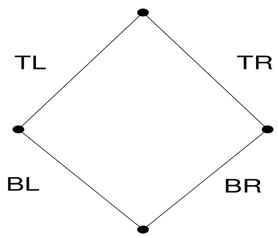

Figure 3. Labelling of C_4.

The following result is an easy consequence of Lemma 2.1 and 2. 2.

Lemma 4.1. *The strong chromatic index of* $C_4C_8(R)[2m;2n]$ *is at least 6.*

4.1 Algorithm for $C_4C_8(R)[2m;2n]$ nanosheet

Input: $C_4C_8(R)[2m;2n]$ nanosheet
Algorithm:
Step 1: Color obtuse edge-cuts of Row *i*,*i* odd of C_4, sequentially as 3,1, 6,5, 3,1, 6,5....
Step 2: Color obtuse edge-cuts of Row *i*,*i* even of C_4, sequentially as 5,6, 1,3, 5,6, 1,3....
Step 3: Color acute edge-cuts of Row *i*,*i* odd of C_4, sequentially as 5,6,1,3, 5,6,1,3....
Step 4: Color acute edge-cuts of Row *i*,*i* even of C_4, sequentially as 3,1,6,5, 3,1,6,5....
Step 5: Color the horizontal edge-cuts as 2.
Step 6: Color the vertical edge-cuts as 4. See Figure 4.
Output:$\chi_s'(C_4C_8(R)[2m;2n]) = 6$.
Proof of correctness: Let G be $(C_4C_8(R)[2m;2n]$ nanosheet. Paths of length 3 in G are of the following category.
1. The 3 edges are distinct members of the set $X = \{a, o, v, h\}$.
2. One edge is acute and the other two are obtuse.
3. One edge is obtuse and the other two are acute.
In all three cases the edges receive distinct colors.

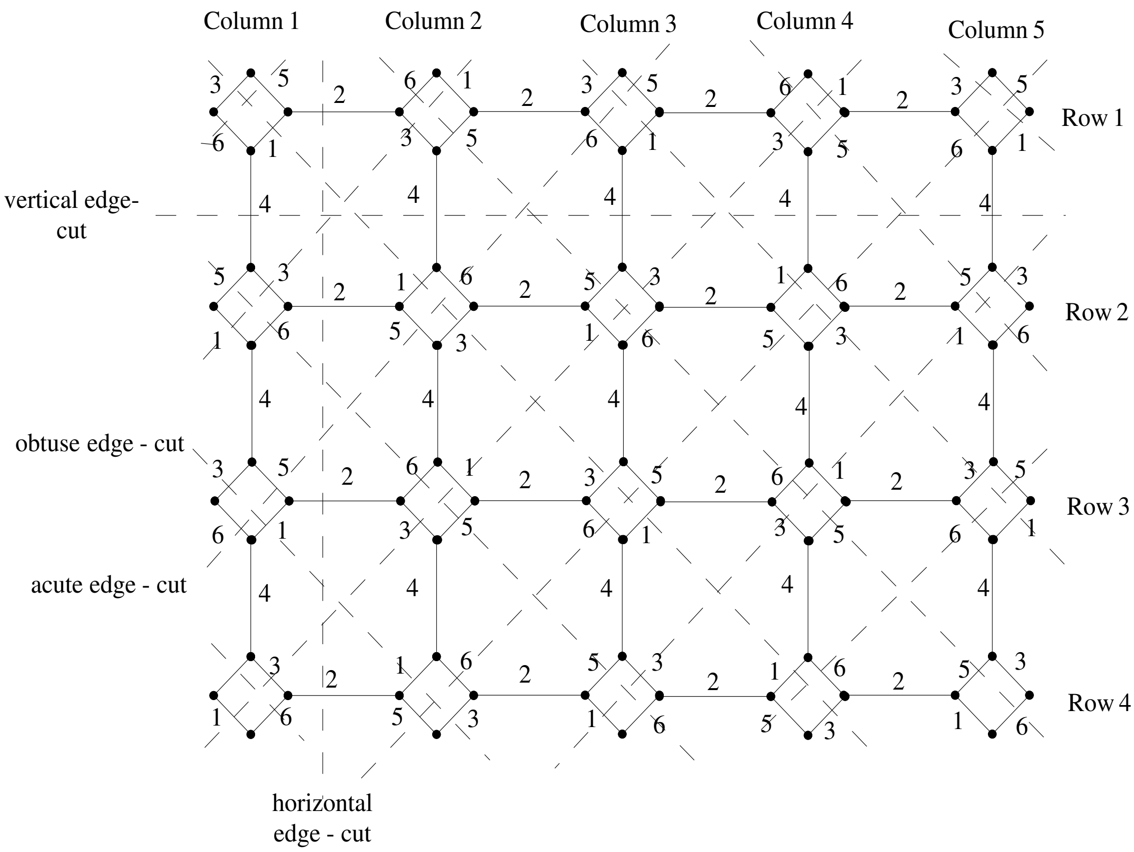

Figure 4. Strong edge-coloring of $C_4C_8(R)[8,10]$ nanosheet.

The following theorem is an easy consequence of Lemma 4.1 and the Algorithm 4.1.

Theorem 4.2. *Let G be a* $C_4C_8(R)[2m;2n]$ *nanosheet. Then* $\chi'_s(G) = 6$.

5 $C_4C_6C_8[2m;2n]$ 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 [19]. The following result is an easy consequence of Lemma 2.5 and Lemma 2.6.

Lemma 5.1. *The strong chromatic index of* $C_4C_6C_8[2m;2n]$ *is at least 6.*

5.1 Algorithm for $C_4C_6C_8[2m;2n]$ nanosheet

Input: $C_4C_6C_8[2m;2n]$ nanosheet
Algorithm:

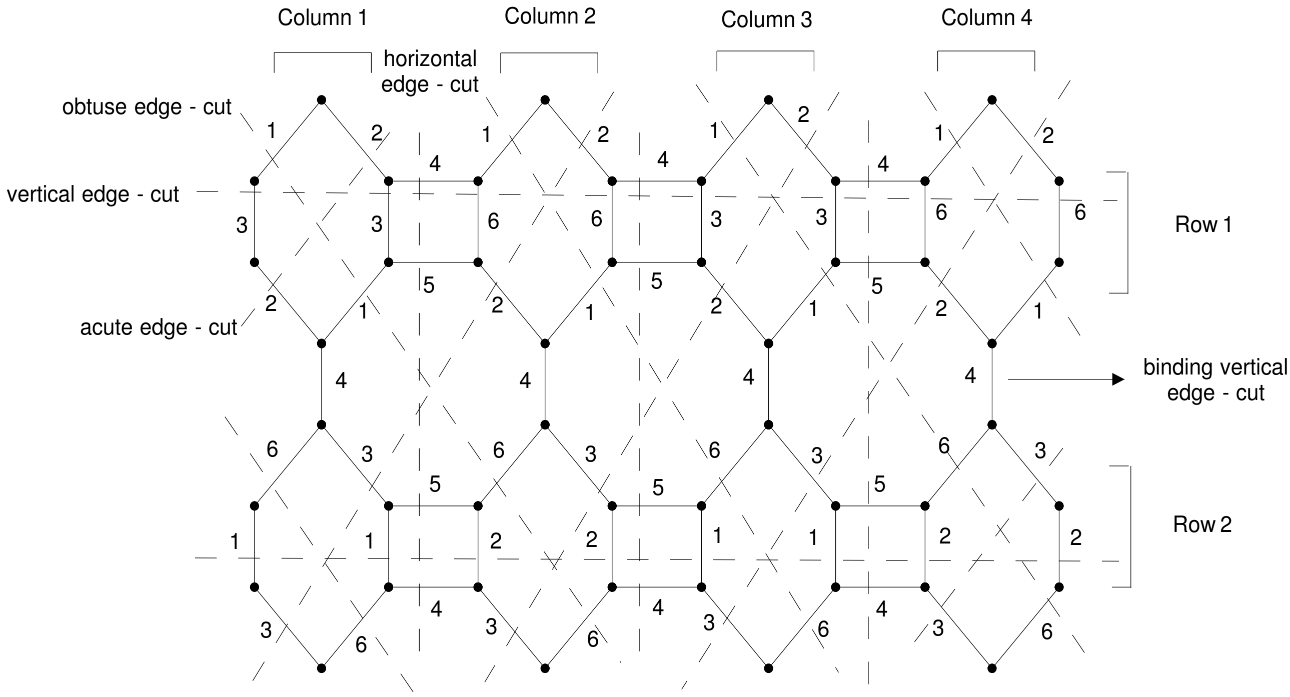

Figure 5. Strong edge-coloring of $C_4C_6C_8[4,6]$ nanosheet.

Step 1: Color obtuse edge-cuts, sequentially as 1,1,6,6, 1,1,6,6. . . .
Step 2: Color acute edge-cuts, sequentially as 2,2,3,3, 2,2,3,3. . . .
Step 3: Color vertical edge-cuts of Row i, i odd, sequentially as 3,3, 6,6, 3,3,. . . .
Step 4: Color vertical edge-cuts of Row i, i even, sequentially as 1,1,2,2,1,1,. . . .
Step 5: Color horizontal edge-cuts as sequentially 4,5,5,4,4,5.
Step 6: Color binding vertical edge-cuts as 4. See Figure 5.
Output:$\chi_s'(C_4C_6C_8[2m;2n]) = 6$.
Proof of correctness: Let G be $(C_4C_6C_8[2m;2n]$ nanosheet. Paths of length 3 in G are of the following category.
1. The 3 edges are distinct members of the set $X = \{a,o,v,h\}$.
2. One edge is horizontal and the other two are vertical.
3. One edge is vertical and the other two are horizontal.
4. One edge is binding horizontal and the other two are obtuse and acute.
In all four cases the edges receive distinct colors.

The following theorem is an easy consequence of Lemma 5.1 and the Algorithm 5.1.

Theorem 5.2. *Let G be a* $C_4C_6C_8[2m;2n]$ *nanosheet. Then* $\chi_s'(G) = 6$.

6 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 [5].

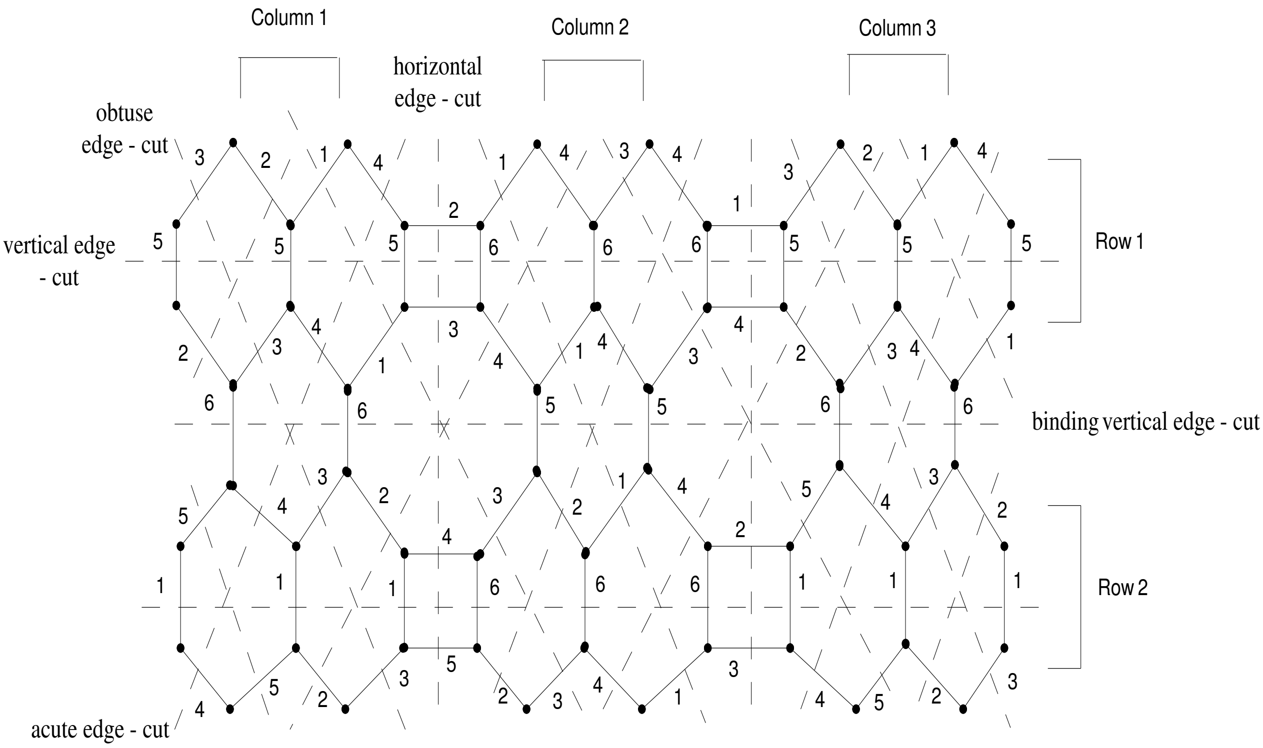

Figure 6. Strong edge-coloring of H -Naphtalenic [2m,2n] Nanosheet

The following result is an easy consequence of Lemma 2.5 and Lemma 2.6.

Lemma 6.1. *The strong chromatic index of H -Naphtalenic $[2m, 2n]$ is at least 6.*

6.1 Algorithm for H -naphtalenic $[2m, 2n]$ nanosheet

Input: H -naphtalenic $[2m, 2n]$ nanosheet
Algorithm:
Step 1: Color obtuse edge-cuts of Row i, i odd, sequentially as 3, 1, 1, 3, 3, 1, 1, 3.
Step 2: Color obtuse edge-cuts of Row i, i even, sequentially as 5, 3, 3, 1, 5, 3, 3, 1.
Step 3: Color acute edge-cuts of Row i, i odd, sequentially as 2, 4, 4, 2, 2, 4, 4, 2.
Step 4: Color acute edge-cuts of Row i, i even, sequentially as 4, 2, 2, 4, 4, 2, 2, 4.
Step 5: Color horizontal edge-cuts of Column i, i odd, sequentially as 2, 3, 4, 5.
Step 6: Color horizontal edge-cuts of Column i, i even, sequentially as 1, 4, 2, 3.
Step 7: Color vertical edge-cuts of Row i, i odd, sequentially as 5, 5, 5, 6, 6, 6, 5, 5, 5.
Step 8: Color vertical edge-cuts of Row i, i even, sequentially as 1, 1, 1, 6, 6, 6, 1, 1, 1.
Step 9: Color binding vertical edge-cuts, sequentially as 6, 6, 5, 5, 6, 6. See Figure 6.

Output:$\chi_s'(\text{H}-naphtalenic[\text{2m,2n}]) = 6$.
Proof of correctness: Let G be H -naphtalenic $[2m, 2n]$ nanosheet. The proof is similar to the nanosheet $C_4C_6C_8[2m, 2n]$.

The following theorem is an easy consequence of Lemma 6.1 and the Algorithm 6.1.

Theorem 6.2. *Let G be a H -naphtalenic* $[2m, 2n]$ *nanosheet. Then* $\chi_s'(G) = 6$.

7 Conclusion

In this paper we developed an algorithms for strong edge-coloring of certain nanosheets using optimum number of colors.

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