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AVD-CHROMATIC INDEX OF $C_5C_7[p, q]$ AND $C_5C_6C_7[p, q]$ NANOTUBES

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Abstract

For a simple connected graph G, adjacent vertex distinguishing (AVD) chromatic index is signified by $\chi'_{AVDCI}(G)$ is indicated as the minimum number r required in coloring of an edge such that no two couple of adjoining vertices have the same set of colors (i.e.) adjacent vertices are differentiated by their color set. In this paper, AVD-Edge coloring is obtained for $C_5C_7[p, q]$ and $C_5C_6C_7[p, q]$ nanotubes.

1. Introduction

Chemical graph theory finds its applications in modeling chemical structures. Graph representation of molecular structure is widely used in computational chemistry [2, 8] and in the study of relationships established by pattern of molecular atomic bonds. Using chemical structures as graphs where vertices are atoms in the molecules and bonds are taken as edges, has gained new attraction and become new methodology in chemistry which helps in the understanding of structures and reactivity. The edge colorings of graphs are functional in multiple quantum Nuclear Magnetic Resonance (NMR) from which various types of dipolor couplings available in molecule is obtained. The edge coloring in graphs are shown to enumerate unique dipolar links among a given set of nuclei there by producing a technique for structure elucidation from NMR [3, 8].

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Let $G = (V, E)$ be a graph with vertex set V and edge set E. A proper edge coloring is a mapping $f : E \to N$ satisfying $f(xy) \neq f(yz)$ for any $xy, yz \in E$. For any $x \in V$, let $C(x)$ signify the set of colors of all edges incident to x. A proper edge coloring f is said to vertex distinguishing if $C(x) \neq C(y)$, for any $x, y \in V$ and $x \neq y$. Adjacent vertex distinguishing edge coloring is a relaxed version of vertex distinguishing in which only adjacent vertices are differentiated by their color set. Mathematically, an adjacent vertex distinguishing chromatic index is a proper edge coloring f satisfying $C(x) \neq C(y)$ for any x, y with $xy \in E$. The minimum number of colors r required for any AVD-edge coloring of G is called r-adjacent vertex distinguishing chromatic index of G and is designated by $\chi'_{AVDCI}(G)$ [6].

Nanotechnology is indicated as the design, characterization, production and application of structures, systems and devices by controlling size and shape at $10^{-9}m$ scale or the single atomic level. Nanotubes are the one of the most widespread studied and used materials consisting of tiny cylinders of carbon and other materials like boron nitride. Carbon nanotubes are allotropes of carbon of a nanostructure having a length to diameter ratio greater than 1,000,000 when graphite sheets are rolled into cylinders their edge are joined together to construct nanotubes. It finds its application in fabric industry, water purification, automobiles, food, energy sector, electronics, Bio-materials and many other fields [3, 9, 10].

Vertex distinguishing proper edge coloring of graphs was first scrutinized by Burris and Schelp [7] and further extended to adjacent vertex distinguishing chromatic index by Balister et al. [4, 5] Zhang et al. [13]. AVD-edge coloring is also studied in the name of adjacent strong edge coloring and 1-strong edge coloring [11]. Here, AVD-chromatic index is obtained for $C_5C_7[p, q]$ and $C_5C_6C_7[p, q]$ nanotubes.

2. Nanotubes with AVD-Edge Coloring

The wrap-around edges in nanotubes are cut to form nanosheets. Nanosheets of carbon compound are a new way of two dimensional polymeric material that is counterfiet by cross linking aromatic self-assembled monolayers with electrons. Due to their constant thickness of only about one nanometer, as well as their high chemical, mechanical and thermal stability, j such materials are fascinating for a wide variety of applications. As the nanosheet is steady under an electron beam, patterns can also be written by electron beam induced deposition (EBID). The stability and exibility nature of carbon nanosheet finds its multifold applications in filtration membranes, sensors, sample supports and even conductive coatings [9, 10, 12]. This nanosheets can be redrawn in the brick form.

3. $C_5C_7[p, q]$ Nanosheet

A $C_5C_7[p, q]$ nanosheet is a trivalent trinket made by alternating pentagons c_5 and septagons c_7. In this section, we compute the adjacent vertex distinguishing edge coloring of $C_5C_7[p, q]$. The number of septagons in first row is signified by p. In this nanosheet, the first 3 rows of vertices and edges repeated alternatively, and number of the repetition of the structure is indicated by q. In each period, there are 8_p vertices and p vertices which are joined to the end of the graph. And hence the number of vertices in this nanosheet is equal to $8pq + p[1, 10]$. This nanosheet can be redrawn in the brick form.

Let the vertex set be defined by $V = \{x_{i, j} 0 \leq i \leq 8pq + p,\ j = 1, 2, \ldots\}$. Let H_k be the sequence of horizontal edges defined by,

$$H_r = \begin{cases} \{x_{r,0}, x_{r,1}, x_{r,2}, \ldots, x_{r,2p-1}\}, & r = 0, 3, 6, \ldots, 3q-3; q = 1, 2, 3, \ldots \\ \{x_{r,0}, x_{r,1}, x_{r,2}, \ldots, x_{r,2p+3}\}, & r = 1, 4, 7, \ldots, 3q-2; q = 1, 2, 3, \ldots \\ \{x_{r,0}, x_{r,1}, x_{r,2}, \ldots, x_{r,2p-3}\}, & r = 2, 5, 8, \ldots, 3q-1; q = 1, 2, 3, \ldots \end{cases}$$

Let V_r be the sequence of vertical edges signified by,

$$V_r = \begin{cases} \{(x_{r,1}, x_{r+1,1}), (x_{r,3}, x_{r+1,4}), \ldots, (x_{r,2n-1}, x_{r+1,3n-2})\}, \\ r = 0, 3, 6, \ldots, 3q-3; n = 1, 2, 3, \ldots \\ \{(x_{r,0}, x_{r+1,1}), (x_{r,3}, x_{r+1,4}), \ldots, (x_{r,3n-3}, x_{r+1,3n-2})\} \cup \\ \{(x_{r,2}, x_{r+1,2}), (x_{r,5}, x_{r+1,5}), \ldots, (x_{r,3n-1}, x_{r+1,3n-1})\} \\ r = 1, 4, 7, \ldots, 3q-2; n = 1, 2, 3, \ldots \\ \{(x_{r,0}, x_{r+1,0}), (x_{r,3}, x_{r+1,2}), \ldots, (x_{r,3n-3}, x_{r+1,2n-2})\} \\ r = 2, 5, 8, \ldots, 3q-1; n = 1, 2, 3, \ldots \end{cases}$$

Theorem 3.1. *Let G be* $c_5c_7[p, q]$ *nanosheet. Then* $\chi'_{AVDCI}(G) = 5$.

Proof. We define the coloring f of horizontal edges H_r as $f(H_1) = (1, 2, 1, 2, \ldots)$, $f(H_2) = (2, 3, 4, 2, 3, 4, \ldots)$, $f(H_3) = (3, 4, 0, 3, 4, 0, \ldots)$, $f(H_i) = (f(H_{i-3}) - 1) \bmod 5$, $\forall 4 \le i \le H_r$.

The coloring f of vertical edges V_r are defined by, $f(V_1) = (0, 0, 0, \ldots)$, $f(V_2) = (1, 1, 1, \ldots)$, $f(V_3) = (2, 2, 2, \ldots)$, $f(V_i) = (f(V_{i-3}) - 1) \bmod 5$, $\forall 4 \le i \le V_r$.

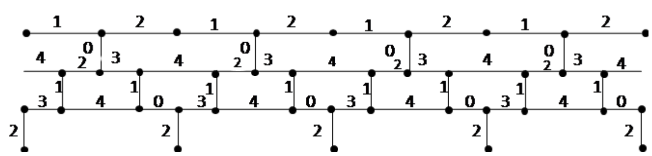

Figure 1. AVD -Edge Coloring of $C_5C_7[4, 1]$.

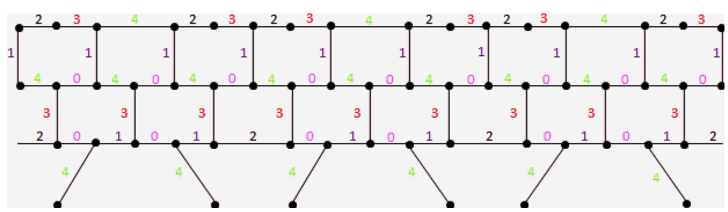

Figure 2. AVD -Edge Coloring of $C_5C_6C_7[3, 1]$.

By construction f is a proper coloring. It stays to show that f is an AVD-edge coloring.

Case 1. For any $x, y \in V$ if $\deg(x) \neq \deg(y)$ then, $C(x) \neq C(y)$. Thus, we only have to compare the sets of colors of adjacent vertices of the same degree.

Case 2. Degree 2 vertices: There are no 2 degree vertices on the upper boundary (horizontal edge) of the graph that are adjacent. Hence they have different set of colors.

Case 3. Degree 3 vertices: There are no three degree vertices that are adjacent in the graph defined by the color set

$$H_0 = C(x_{i,j}) = (\alpha, \alpha + 1, \beta) = (1, 2, 0) \bmod 5$$

$$H_1 = \begin{cases} C(x_{i+1, 3j-2}) = (\alpha + 1, \alpha + 2, \beta) \bmod 5 & i = 0, 1, 2, \ldots, j = 1, 2, 3, \ldots \\ C(x_{i+1, 3j-3}) = (\alpha + 3, \alpha + 1, \beta + 1) \bmod 5 & i = 0, 1, 2, \ldots, j = 1, 2, 3, \ldots \\ C(x_{i+1, 3j-1}) = (\alpha + 2, \alpha + 3, \beta + 1) \bmod 5 & i = 0, 1, 2, \ldots, j = 1, 2, 3, \ldots \end{cases}$$

$$H_2 = \begin{cases} C(x_{i+2, 3j-2}) = (\alpha + 2, \alpha + 3, \beta + 1) \bmod 5 & i = 0, 1, 2, \ldots, j = 1, 2, 3, \ldots \\ C(x_{i+2, 3j-1}) = (\alpha + 4, \alpha + 3, \beta + 1) \bmod 5 & i = 0, 1, 2, \ldots, j = 1, 2, 3, \ldots \\ C(x_{i+2, 3j-3}) = (\alpha + 4, \alpha + 2, \beta + 2) \bmod 5 & i = 0, 1, 2, \ldots, j = 1, 2, 3, \ldots \end{cases}$$

From this it follows $C(x_{i+1, 3j-2}) \neq C(x_{i+1, 3j-3}) \neq C(x_{i+1, 3j-1})$ and $C(x_{i+2, 3j-2}) \neq C(x_{i+2, 3j-1}) \neq C(x_{i+2, 3j-1})$ as shown in Figure 1. □

4. $C_5C_6C_7[p, q]$ Nanosheet

A $C_5C_6C_7[p, q]$ nanosheet is a trivalent decoration made by alternating pentagons c_5 and C_6 septagons c_7. In this section, we compute the adjacent vertex distinguishing edge coloring of $C_5C_6C_7[p, q]$. The number of pentagons in first row is denoted by p. In this nanosheet, the first 3 rows of vertices and edges repeat alternatively, and number of the repetition of the structure is denoted by q called period. In each period, there are $16p$ vertices and $2p$ vertices which are joined to the end of the graph. And hence the number of vertices in this nanosheet is equal to $16pq + 2p[1, 10]$. This nanosheet can be redrawn in the brick form.

Let the vertex set be defined by $V = \{x_{i,j} 0 \leq i \leq 16pq + 2p,\ j = 1, 2, \ldots,\}$.

Let H_k be the sequence of horizontal edges defined by,

$$H_r = \begin{cases} \{x_{r,0}, x_{r,1}, x_{r,2}, \ldots, x_{r,5p-1}\}, & r = 0, 3, 6, \ldots, 3q-1 \\ \{x_{r,0}, x_{r,1}, x_{r,2}, \ldots, x_{r,6p-1}\}, & r = 1, 4, 7, \ldots, 3q \\ \{x_{r,0}, x_{r,1}, x_{r,2}, \ldots, x_{r,5p-1}\}, & r = 2, 5, 8, \ldots, 3q+1 \end{cases}.$$

Let $V_r,\ V_r' V_r''$ be the sequence of vertical edges defined by,

$$V_r = \begin{cases} \{(x_{r,0}, x_{r+1,0}), (x_{r,5}, x_{r+1,6}), \ldots, (x_{r,5n-5}, x_{r+1,6n-6})\} \cup \\ \{(x_{r,2}, x_{r+1,2}), (x_{r,7}, x_{r+1,8}), \ldots, (x_{r,5n-3}, x_{r+1,6n-4})\} \cup \\ \{(x_{r,3}, x_{r+1,4}), (x_{r,8}, x_{r+1,10}), \ldots, (x_{r,5n-2}, x_{r+1,6n-2})\} r = 0, 3, 6, \\ \{(x_{r,1}, x_{r+1,0}), (x_{r,7}, x_{r+1,5}), \ldots, (x_{r,6n-5}, x_{r+1,5n-5})\} \cup \\ \{(x_{r,3}, x_{r+1,2}), (x_{r,9}, x_{r+1,7}), \ldots, (x_{r,6n-3}, x_{r+1,5n-1})\} r = 1, 4, 7, \ldots \\ \{(x_{r,1}, x_{r+1,1}), (x_{r,6}, x_{r+1,6}), \ldots, (x_{r,5n-4}, x_{r+1,5n-4})\} \cup \\ \{(x_{r,3}, x_{r+1,4}), (x_{r,8}, x_{r+1,9}), \ldots, (x_{r,5n-2}, x_{r+1,5n-1})\} r = 2, 5, 8, \ldots \end{cases}$$

for $n = 1, 2, 3, \ldots$.

Theorem 4.1. *Let G be* $C_5C_6C_7[p, q]$ *nanosheet. Then* $\chi'_{AVDCI}(G) = 5$.

Proof. We define the coloring c of horizontal edges H_r. $f(H_1) = (2, 3, 4, 2, 3, 2, 3, 4, \ldots)$, $f(H_2) = (4, 0, 4, 0, \ldots)$, $f(H_3) = (3, 4, 0, 3, 4, 0, \ldots,)$, $f(H_i) = (c(H_{i-3}) - 1) \bmod 5,\ \forall\ 4 \leq i \leq H_k$.

The coloring f of vertical edges V_r defined by, $f(V_1) = (1, 1, 1, \ldots)$, $f(V_2) = (3, 3, 3, \ldots)$, $f(V_3) = (4, 4, 4, \ldots)$. The same coloring repeats in each period.

By construction f is a proper coloring. It remains to show that f is an

AVD-edge coloring.

Case 1. For any $x, y \in V$ if $\deg(x) \neq \deg(y)$ then, $C(x) \neq C(y)$. Thus, we only have to compare the sets of colors of adjacent vertices of the same degree.

Case 2. Degree 2 vertices: There are no 2 degree vertices on the upper boundary (horizontal edge) of the graph that are adjacent. Hence they have different set of colors.

Case 3. Degree 3 vertices: Here no two 3 degree vertices are adjacent on the upper border of the graph G. Let $C(x_{i,j}) = (\alpha, \alpha+1, \beta)$. Let

$$H_0 = \begin{cases} C(x_{i,5j-3}) = (\alpha, \alpha+1, \beta) \bmod 5 \\ C(x_{i,5j-2}) = (\alpha+1, \alpha-1, \beta) \bmod 5 \\ C(x_{i,5j}) = (\alpha, \alpha-1, \beta) \bmod 5 \; i = 0, 3, 6, \ldots \end{cases}$$

$$H_1 = \begin{cases} C(x_{i+1,2j-1}) = (\alpha+1, \alpha+2, \beta+2) \bmod 5 \\ C(x_{i+1,2j}) = (\alpha+2, \alpha+1, \beta) \bmod 5 \end{cases}$$

$$H_2 = \begin{cases} C(x_{i+2,5j-5}) = (\alpha-1, \alpha+2, \beta+2) \bmod 5 \\ C(x_{i+2,5j-4}) = (\alpha+2, \alpha-2, \beta+1) \bmod 5 \\ C(x_{i+2,5j-3}) = (\alpha-2, \alpha+2, \beta) \bmod 5 \\ C(x_{i+2,5j-2}) = (\alpha+2, \alpha-2, \beta-2) \bmod 5 \\ C(x_{i+2,5j-1}) = (\alpha-2, \alpha+1, \beta+2) \end{cases}$$

Hence $C(x_{i,5j-3}) \neq C(x_{i,5j-2}) \neq C(x_{i,5j})$, $C(x_{i+1,j-1}) \neq C(x_{i+1,2j})$ and $C(x_{i+2,5j-5}) \neq C(x_{i+2,5j-4}) \neq C(x_{i+2,5j-3}) \neq C(x_{i+2,5j-2}) \neq C(x_{i+2,5j-1})$ as shown in Figure 2. □

5. Conclusion

Here, we have proved that AVD-edge coloring of $C_5C_7[p, q]$ nanosheet and $C_5C_6C_7[p, q]$ nanosheet is $\Delta(G) + 2$.

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