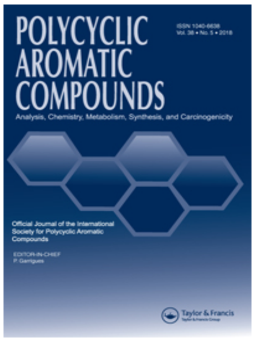

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Excessive Index of Certain Carbon Based Nanotubes

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ABSTRACT

Chemical graph theory models have been extensively used as predictors of the properties of chemical compounds. Nanotechnology is the study of manipulating matter on an atomic and molecular scale. There are many applications of nanotechnology in the area of medicine, chemistry, energy, agriculture, information and communication, heavy industry, and consumer goods. A Kekule structure in a molecular graph is nothing but a perfect matching in the graph. The minimum number of Kekule structures that cover the edge set of a molecular graph G is known as the excessive index of G. In this article, we determine the excessive index for $TUC_4C_8(S)[p,q]$ nanosheet, $NPHX[m,n]$ nanotube, $TUC_4C_8(R)[p,q]$ nanotube, H-anthracenic nanotube, and H-tetracenic nanotube.

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Kekule structures; perfect matchings; excessive index carbon based nanotubes

Introduction

The structure of benzene as a six-membered ring of carbon atoms was introduced by the German chemist F. A. Kekule in 1865. To make the structure compatible with the quadriyalence of carbon, he introduced alternating single and double bonds in the ring. The usual structural representation for benzene is a six carbon ring (represented by a hexagon) which includes three double bonds. Each of the carbons represented by a corner is also bonded to one other atom. In benzene the double bonds are separated by single bonds so we recognize the arrangement as involving conjugated double bonds. In 1991, Iijima discovered a complex, elongated type of fullerene: the carbon nanotube (CNT) it can be imagined as a C_{70} fullerene with many thousands of carbon rings inserted across its equator, giving a tiny tube with about 1.5 nm of diameter and a length of several microns. Like graphite, CNTs are also composed of sp^2 carbons, meaning that each carbon is engaged in a single double (C–C) bond and two single (C–C) bonds. Therefore CNTs, like graphite, pyrene, coronene, and many other hexagonal systems immersed in the "sea" of π-electrons, are also benzenoid systems. The stability of benzenoids may be approximated by determining the Kekule' structure count (K) that is the number of ways the double bonds can be placed in the chemical graph consisting of hexagons. A dominant role is played by three sciences: mathematics, chemistry, and computer science. Models presented here give an insight into the nature of some chemical compounds. The most interesting feature of these models is the possibility to predict the properties of chemical compounds that have never existed nor been synthesized. Hence, Kekule theory gives us a glimpse beyond our real world, a glimpse into the world of almost infinite possibilities. Nanotube structures have many applications in the general field of nanotechnology, which is a relatively recent field with much potential, as well as some significant liabilities. The engineering of molecular products needs to be carried out by robotic devices, which have been termed nanorobots.[1] Nanorobotics is a field which calls for collaborative efforts between physicists, chemists, biologists, computer scientists, engineers, and other specialists.[2–6] Currently

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this field is still evolving, but several substantial steps have been taken by great researchers all over the world contributing to this ever challenging and exciting field. The field of nanorobotics studies the design, manufacturing, programming, and control of the nanoscale robots. Controlling nanoscale robot is obtained by proper scheduling. Scheduling is the process of deciding how to commit resources between a variety of possible tasks. Carbon nanotubes consist of carbon atoms bonded into a tube shape where carbon atoms are located at apexes of regular hexagons on two-dimensional surfaces. Carbon nanotubes are extremely strong, probably one of the strongest materials that is even theoretically possible. Determining excessive index has important applications in scheduling.[7] Structures realized by arrangements of regular hexagons in the plane are of interest in the chemistry of benzenoid hydrocarbons, where perfect matchings correspond to kekule structures which feature in the calculation of molecular energies associated with benzenoid hydrocarbon molecules.[8] Chemical graph theory is a subdivision of mathematical chemistry in which we apply tools of graph theory to represent the chemical phenomenon mathematically. Chemical graphs are models of molecules in which atoms are represented by vertices and chemical bonds by edges of a graph. For a graph G let $V(G)$ denotes the set of vertices in G, $E(G)$ denotes the set of edges in G, $|V(G)|$ and $|E(G)|$ denote the respective cardinalities of these sets. The *degree* or *valency* $d_G(v)$ of a vertex v in G is the number of edges of G incident with v, each loop counted as two edges. The maximum degree of G denoted by $\Delta(G)$, is the degree of the vertex with the greatest number of edges incident to it. The minimum degree of G denoted by $\delta(G)$, is the degree of the vertex with the least number of edges incident to it. For each vertex $v \in V$, the *open neighborhood* of v is the set $N(v)$ containing all the vertices u adjacent to v and the closed neighborhood of v is the set $N(v) = N(v) \cup \{v\}$. A matching in a graph $G = (V, E)$ is a subset M of edges, no two of which have a vertex in common. A matching M is said to be perfect if every vertex in G is an endpoint of one of the edges in M. Thus a perfect matching in G is a 1-regular spanning subgraph of G. An almost perfect matching or near 1-factor matching covers all but exactly one vertex. A graph G is 1-extendable if every edge of G belongs to at least one 1-factor of G. A 1-factor cover of G is a set $\mathcal{F}$ of 1-factors of G such that $\cup_{F\in\mathcal{F}} F = E(G)$. A 1-factor cover of minimum cardinality is called an excessive factorization.[9,10] The excessive index of G, denoted $\chi'_e(G)$ is the size of an excessive factorization of G and defined $\chi'_e(G) = \infty$ if G is not 1-extendable. A graph G is 1-factorizable if its edge set $E(G)$ can be partitioned into edge-disjoint 1-factors. An excessive near 1-factorization of a graph G is a minimum set of near 1-factors whose union contains all the edges of G.[11,12] Excessive index has a number of applications particularly in scheduling theory to complete the process in minimum possible time.[12] In the literature the problem of determining whether a regular graph G is 1-factorizable is NP-complete.[13] The objective and basic concept of the manuscript is to determine the excessive index for $TUC_4C_8(S)[p,q]$ nanosheet, $NPHX[m,n]$ nanotube, $TUC_4C_8(R)[p,q]$ nanotube, H-anthracenic nanotube and H-tetracenic nanotube.

Theorem 1.1. [14] *Let G be a graph. Then* $\chi'_e(G) \geq \Delta$.

Theorem 1.2. [14] *Let G be a regular graph with even order. Then* $\chi'_e(G) = \Delta$ *if and only if G is 1-factorizable.*

Theorem 1.3. [15] *Let G be a graph of order n with* $\delta = 2$. *Let* $v_1, v_2, \ldots, v_m$, $m < n$, *be the vertices of degree 2 in G. Suppose* $N(v_i) = \{ v_i^1, v_i^2 \}$, $1 \leq i \leq m$, $\deg(v_i^1) = k_i^1 + 1$ *and* $\deg(v_i^2) = k_i^2 + 1$, *then* $\chi'_e(G) \geq max_i\{k_i^1 + k_i^2\}$, $1 \leq i \leq m$.

Lemma 1.4. *Let G be a graph which is connected,* $|G| = n$ *with* $\delta = 2$. *Let* $v_1, v_2, \ldots, v_m$, $m < n$, *be the vertices of degree 2 in G. Suppose* $N(v_1) = \{ v_1^1, v_1^2 \}, N(v_2) = \{ v_2^1, v_2^2 \}, \ldots, N(v_i) = \{ v_i^1, v_i^2 \}$, $1 \leq i \leq m$ *and* $N(v_1 \cap v_2) = r_1$, $N(v_2 \cap v_3) = r_2, \ldots$, $N(v_{i-1} \cap v_i) = r_j$, $1 \leq i \leq m$, $1 \leq j \leq m -$

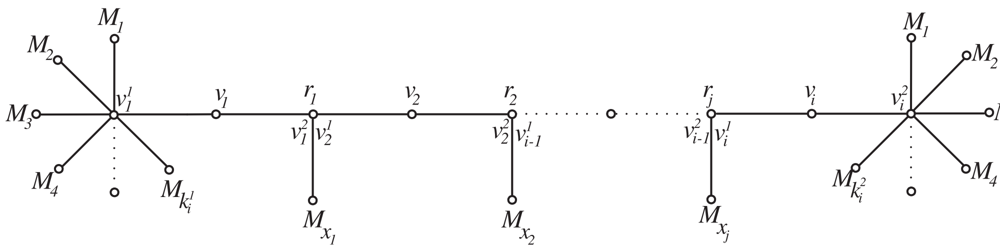

Figure 1. The graph *G*.

1. $\deg(v_1^1) = k_i^1 + 1, \deg(r_1) = x_1 + 2, \deg(r_2) = x_2 + 2, \ldots, \deg(r_j) = x_j + 2, \deg(v_i^2) = k_i^2 + 1$ *then* $\chi_e'(G) \geq max\{k_i^1 + k_i^2\} + \cup_{p=1}^{j} x_p$, $1 \leq i \leq m$, $1 \leq j \leq m - 1$.

Proof. Consider the 2 degree vertex v_1. Let $M_1, M_2, \ldots, M_{k_i^1}$ be the perfect matchings that cover all the edges incident at v_1^1 other than $v_1^1 v_1$ and let $M_1, M_2, \ldots, M_{k_i^2}$ be the perfect matchings that cover all the edges incident at v_i^2 other than $v_i^2 v_i$. Then the edge $v_1 v_1^1$ is in every M_s, $1 \leq s \leq k_i^1$ and the edge $v_i v_i^2$ is in every M_s, $1 \leq s \leq k_i^2$. Clearly x_j number of distinct perfect matchings other than $M_1, M_2, \ldots, M_{k_i^1}$ and $M_1, M_2, \ldots, M_{k_i^2}$ are necessary to cover the edges incident at r_j, $1 \leq j \leq m - 1$. See Figure 1. This implies $\chi_e'(G) \geq max\{k_i^1 + k_i^2\} + \cup_{p=1}^{j} x_p$, where the maximum is taken over all i, j, $1 \leq i \leq m$, $1 \leq j \leq m - 1$. □

Excessive index of $TUC_4C_8(S)[p, q]$ nanosheet

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. 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.[16] Consider the molecular graph of an $TUC_4C_8(S)[p, q]$ nanosheets. Let $G = TUC_4C_8(S)[p, q]$ where p is the number of rows and q is the number of columns. $TUC_4C_8(S)$ nanosheets is bi-regular graph. See Figure 2.

Theorem 2.1. *Let G be the* $TUC_4C_8(S)[p, q]$ *nanosheet, then* $\chi_e'(G) = 3$.
Proof. By Theorem 1.1 $\chi_e'(G) \geq 3$. We now proceed to prove that the lower bound is sharp. Let us construct three perfect matchings M_1, M_2 and M_3 covering all the edges of $TUC_4C_8(S)[p, q]$ nanosheet. Perfect matchings M_1, M_2 and M_3 are selected as follows: Let M_1 be the perfect matching consists of acute and obtuse edges in octagons. Let M_2 be the perfect matching consists of all vertical edges in both octagon and squares together with the horizontal edges on the boundary. Let M_3 be the perfect matching consists of all horizontal edges in both octagon and squares together with the vertical edges on the boundary. Clearly the edges in M_1, M_2 and M_3 are selected in such a way that each $M_i, 1 \leq i \leq 3$ is perfect. This implies that $M_1 \cup M_2 \cup M_3$ cover all the edges of G. Thus $\chi_e'(G) = 3$. □

Excessive index of $TUC_4C_8(R)[p, q]$ nanotube

In this section, we compute the excessive index for $TUC_4C_8(R)[p, q]$ nanotube. Consider the molecular graph of an $TUC_4C_8(R)$ nanotube. $T[p, q]$ denotes a $TUC_4C_8(R)$ nanotube parameterized by the number of octagons in a fixed row (p) and column (q) of a 2-dimensional lattice such as shown in Figure 3. The nanotube is obtained from the lattice by wrapping it up so that each

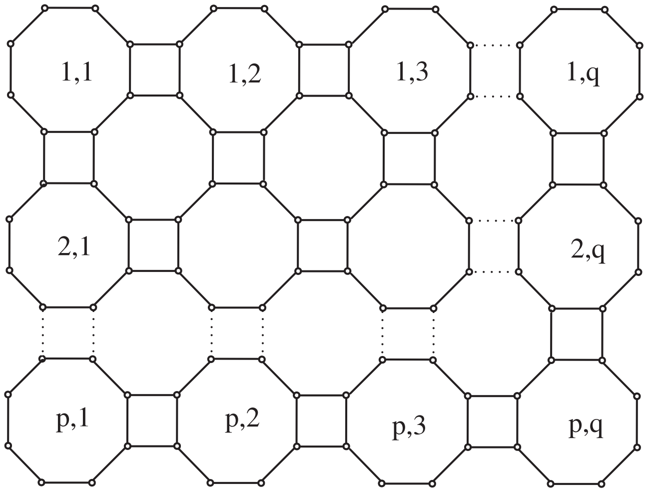

Figure 2. $TUC_4C_8(S)[p,q]$ nanosheet.

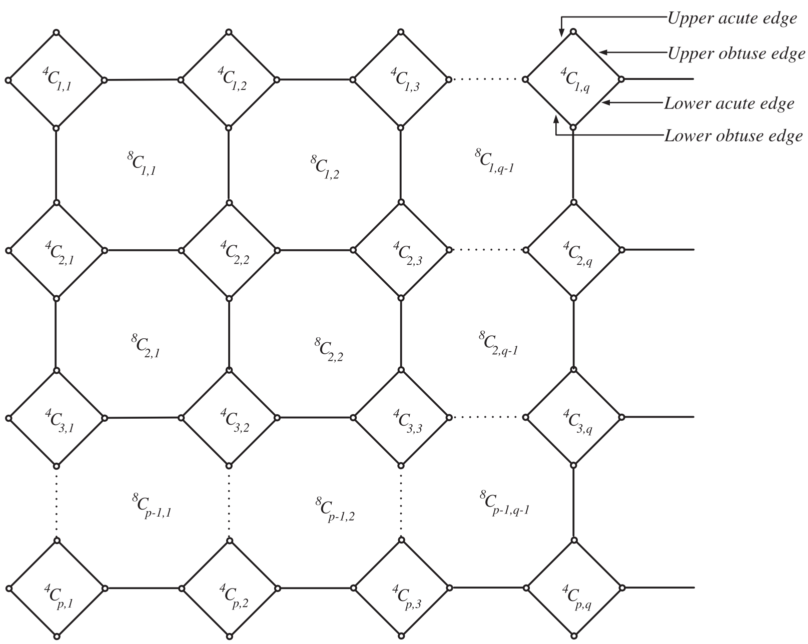

Figure 3. $TUC_4C_8(R)[p,q]$ nanotube.

dangling edges from the left hand side connects to the rightmost vertex of the same row. The number of both squares and octagons in one layer of the nanotube is equal to $p+1$. As each vertex of $TUC_4C_8(R)$ nanotube is contained in exactly one square, the structure $TUC_4C_8(R)[p;q]$ has $(4+1)(q+1)$ vertices and $(p+1)(6q+5)$ edges. The $TUC_4C_8(R)$ nanotube is bi-regular graph.[17]

Theorem 3.1. *Let G be the $TUC_4C_8(R)$ nanotube, then $\chi'_e(G) = 4$.*

Proof. By Lemma 1.3, $\chi'_e(G) \geq 4$. We now proceed to prove that the lower bound is sharp.
Case 1: p- even(odd), q- even

Perfect matchings M_1, M_2, M_3 and M_4 are selected as follows:

Step 1: (Selection of edges in M_1)

a. From $C^4_{1,j}$ select the upper acute edges where j-odd and select the upper obtuse edges where j-even. From $C^4_{p,j}$ select the lower acute edges where j-even (odd) and lower obtuse edges where j- odd (even).
b. Select all the horizontal and vertical edges of $C^8_{i,j}$ where i, j-odd and i, j-even.

Step 2: (Selection of edges in M_2)

a. From $C^4_{1,j}$ select the upper acute edges where j-even and select the upper obtuse edges where j-odd. From $C^4_{p,j}$ select the lower acute edges where j-odd (even) and lower obtuse edges where j- even (odd).
b. Select all the horizontal and vertical edges of $C^8_{i,j}$ where i-odd, j-even and i-even, j-odd.

Step 3: (Selection of edges in M_3)
From $C^4_{i,j}$ where $i = 1, 2, ...p, j = 1, 2, ...q$ select all the upper and lower acute edges.
Step 4: (Selection of edges in M_4)
From $C^4_{i,j}$ where $i = 1, 2, ...p, j = 1, 2, ...q$ select all the upper and lower obtuse edges.

Clearly the edges in M_1, M_2, M_3 and M_4 are selected in such a way that each M_i, $1 \leq i \leq 4$ is perfect. Further steps 1 (b) and 2 (b) cover all the horizontal and vertical edges while steps 3 and 4 cover all the acute and obtuse edges.

Case 2: p- even(odd), q- odd

Perfect matchings M_1, M_2, M_3 and M_4 are selected as follows:
Step 1: (Selection of edges in M_1)

a. From $C^4_{1,j}$ select the upper acute edges where j-odd and the upper obtuse edges where j-even. From $C^4_{i,1}$ select the upper acute edges where i-odd and the lower obtuse edges where i-even. From $C^4_{i,q}$ select the lower acute edges where i-odd and the upper obtuse edges where i-even. From $C^4_{p,j}$ select the lower obtuse(acute) edges where j-odd and the lower acute(obtuse) edges where j-even.
b. Select all the horizontal and vertical edges of $C^8_{i,j}$ where i, j-odd, i, j-even, $i = 1, 2, ...p$ and $j = 1, 2, ...(q-1)$.

Step 2: (Selection of edges in M_2)

a. From $C^4_{1,j}$ select the upper obtuse edges where j-odd and the upper acute edges where j-even. From $C^4_{i,1}$ select the lower obtuse edges where i-odd and the upper acute edges where i-even. From $C^4_{i,q}$ select the upper obtuse edges where i-odd and the lower acute edges where i-even. From $C^4_{p,j}$ select the lower acute(obtuse) edges where j-odd and the lower obtuse(acute) edges where j-even.
b. Select all the horizontal and vertical edges of $C^8_{i,j}$ where i, j-odd, even and i, j-even, odd $i = 1, 2, ...p$ and $j = 1, 2, ...(q-1)$.

Step 3: (Selection of edges in M_3)

a. From $C^4_{i,j}$ select all the upper and lower acute edges where $i = 1, 2, ...p, j = 2, 3, ...(q-1)$. From $C^4_{i,1}$ select the upper obtuse edges where i-odd and the lower acute edges where i-even. From $C^4_{i,q}$ select the upper acute edges where i-odd and the lower obtuse edges where i-even. (From $C^4_{p,1}(C^4_{p,q})$ select the upper and lower obtuse(acute) edges.

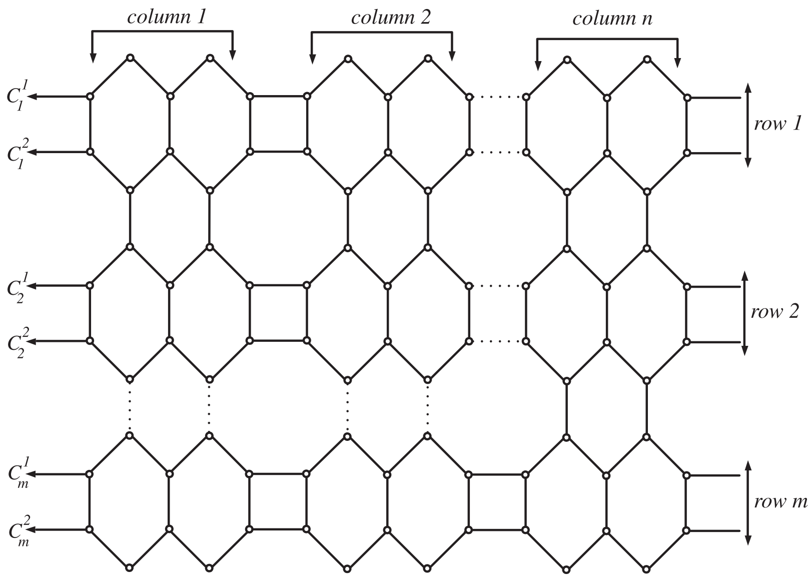

Figure 4. NPHX[m,n] nanotube.

b. From $C^8_{i,q}$ select all the horizontal and vertical edges where i-odd.

Step 4: (Selection of edges in M_4 for p-even)

From $C^4_{i,j}$ select all the upper and lower obtuse edges where $i = 1, 2, \ldots p, j = 2, 3, \ldots (q-1)$. From $C^4_{i,1}$ select the upper and lower acute edges for i-odd and the upper and lower obtuse edges for $i-$ even. From $C^4_{i,q}$ select the upper and lower obtuse edges for i-odd and the upper and lower acute edged for i-even.

(Selection of edges in M_4 for p-odd)

a. From $C^4_{i,j}$ select all the upper and lower obtuse edges where $i = 1, 2, \ldots p, j = 2, 3, \ldots (q-1)$. From $C^4_{i,1}(C^4_{i,q})$ select the upper acute(obtuse) edges for i-odd and the lower obtuse(acute) edges for $i-$ even. From $C^4_{1,1}(C^4_{1,q})$ select the upper and lower acute(obtuse) edges.
b. From $C^8_{i,q}$ select all the horizontal and vertical edges where i-even.

Clearly the edges in M_1, M_2, M_3 and M_4 are selected in such a way that each M_i, $1 \leq i \leq 4$ is perfect.

Further steps 1 (b), 2 (b), 3 (b), and 4 (b) cover all the horizontal and vertical edges while steps 1 (a), 2 (a), 3 (a), and 4 (a) cover all the acute and obtuse edges. Thus $\chi'_e(G) = 4$. □

Excessive index of NPHX[*m*,*n*] nanotube

In this section, we compute the excessive index for H-naphtalenic nanotubes. This nanotube is a trivalent decoration having sequence of C_6, C_6, C_4, C_6, C_6, $C_4, \ldots$ in first row and a sequence of C_6, C_8, C_6, $C_8, \ldots$ in other row. In other words, the whole lattice is a plane tiling of C_6,C_4 and C_8 and this type of tiling can either cover a cylinder or a torus.[18,19] These nanotubes usually symbolized as NPHX[m,n], in which m is the number of pairs of hexagons in first row and n is the number of alternative hexagons in a column as depicted in Figure 4.

Theorem 4.1. *Let G be the NPHX*$[m, n]$ *nanotube, then* $\chi'_e(G) = 5$.

Proof . By Lemma 1.4, $\chi'_e(G) \geq 5$. We now proceed to prove that the lower bound is sharp. **Case 1:** (n-odd)

Perfect matchings M_1, M_2, M_3, M_4 and M_5 are selected as follows:
Step 1: (Selection of edges in M_1)

a. From C_1^1, select the acute edges of column j, j odd and obtuse edges of column j, j even and from C_1^2, select the acute edges of column j, j even and obtuse edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of squares induced by column j and $j+1$, j odd, together with the vertical edges of column n with one end incident at an obtuse edge of C_i^1 and the other end incident at an acute edge of $C_i^2, 1 \leq i \leq m$.

Step 2: (Selection of edges in M_2)

a. From C_1^1, select the obtuse edges of column j, j odd and acute edges of column j, j even and from C_1^2, select the obtuse edges of column j, j even and acute edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of squares induced by column j and $j+1$, j even, together with the vertical edges of column 1 with one end incident at an acute edge of C_i^1 and the other end incident at an obtuse edge of $C_i^2, 1 \leq i \leq m$.

Step 3: (Selection of edges in M_3)

a. From C_1^1 select the acute and obtuse edges of column $j, 1 \leq j \leq n$ and from C_m^2, select the obtuse and acute edges of column $j, 1 \leq j \leq n$.
b. Select the vertical edges from column $j, 1 \leq j \leq n$ with one end incident at an acute and an obtuse edge of $C_i^1(C_i^2)$ with other end incident at an acute and an obtuse edge of $C_i^2(C_{i+1}^1)$ together with the vertical edges of squares in row $i, 1 < i < m$, induced by the columns $j, j+1, 1 \leq j \leq n$ and the horizontal edges of squares incident with the acute and obtuse edges of C_1^2 and C_n^2.

Step 4: (Selection of edges in M_4)

a. From C_1^1, select the obtuse edges of column 1 and the acute edges of column $j, 1 < j \leq n$ and from C_2^1, select the acute edges of column 1 and the obtuse edges of column $j, 1 < j \leq n$. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of the squares induced by column 1 and column n, and the vertical edges of the squares induced by column j and $j+1, 1 < j < n$ with one end incident at an obtuse edge in C_i^1 and the other end incident at an acute edge in $C_i^2, 1 \leq i \leq m$.

Step 5: (Selection of edges in M_5)

a. From C_1^1, select the acute edges of column 1 and the obtuse edges of column $j, 1 < j \leq n$ and from C_2^1, select the obtuse edges of column 1 and the acute edges of column $j, 1 < j \leq n$. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the vertical edges of the squares induced by column 1 and 2, the vertical edges of the squares induced by column j and $j+1, 1 < j < n$ with one end incident at an acute edge in C_i^1 and the other end incident at an obtuse edge in $C_i^2, 1 \leq i \leq m$.

Clearly the edges in M_1, M_2, M_3, M_4 and M_5 are selected in such a way that each $M_i, 1 \leq i \leq 5$ is perfect. Further steps 1 (a), 2 (a) cover all acute and obtuse edges, steps 1 (b), 2 (b), and 4 (b) cover all horizontal edges, steps 1 (b), 2 (b), 3 (b), 4 (b), and 5 (b) cover all vertical edges. Thus $\chi_e'(G) = 5$.

Case 2: (n-even)

Perfect matchings M_1, M_2, M_3, M_4 and M_5 are selected as follows:

Step 1: (Selection of edges in M_1)

a. From C_1^1, select the acute edges of column j, j odd and obtuse edges of column j, j even and from C_1^2, select the acute edges of column j, j even and obtuse edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of squares induced by column j and $j+1$, j odd.

Step 2: (Selection of edges in M_2)

a. From C_1^1, select the obtuse edges of column j, j odd and acute edges of column j, j even and from C_1^2, select the obtuse edges of column j, j even and acute edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of squares induced by column j and $j+1$, j even.

Step 3: (Selection of edges in M_3)

a. From C_1^1 select the acute and obtuse edges of column $j, 1 \leq j \leq n$ and from C_m^2, select the obtuse and acute edges of column $j, 1 \leq j \leq n$.
b. Select the vertical edges from column $j, 1 \leq j \leq n$ with one end incident at an acute and an obtuse edge of $C_i^1(C_i^2)$ with other end incident at an acute and an obtuse edge of $C_i^2(C_{i+1}^1)$ together with the vertical edges of squares in row $i, 1 < i < m$, induced by the columns $j, j+1, 1 \leq j \leq n$ and the horizontal edges of squares incident with the acute and obtuse edges of C_1^2 and C_n^2.

Step 4: (Selection of edges in M_4)

a. From C_1^1, select the obtuse edges of column j for $1 \leq j \leq n$ and from C_2^1, select the acute edges of column j for $1 \leq j \leq n$. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the vertical edges of the squares induced by column j and $j+1, 1 \leq j \leq n$ with one end incident at an acute edge in C_i^1 and the other end incident at an obtuse edge in $C_i^2, 1 \leq i \leq m$.

Step 5: (Selection of edges in M_5)

a. From C_1^1, select the acute edges of column j, $1 \leq j \leq n$ and from C_2^1, select the obtuse edges of column $j, 1 \leq j \leq n$. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the vertical edges of the squares induced by column j and $j+1, 1 \leq j \leq n$ with one end incident at an obtuse edge in C_i^1 and the other end incident at an acute edge in $C_i^2, 1 \leq i \leq m$.

Clearly the edges in M_1, M_2, M_3, M_4 and M_5 are selected in such a way that each $M_i, 1 \leq i \leq 5$ is perfect. Further steps 1 (a), 2 (a) cover all the acute and obtuse edges, steps 1 (b)and 2 (b) cover all the horizontal edges, steps 3 (b), 4 (b), and 5 (b) cover all the vertical edges. Thus $\chi_e'(G) = 5$. □

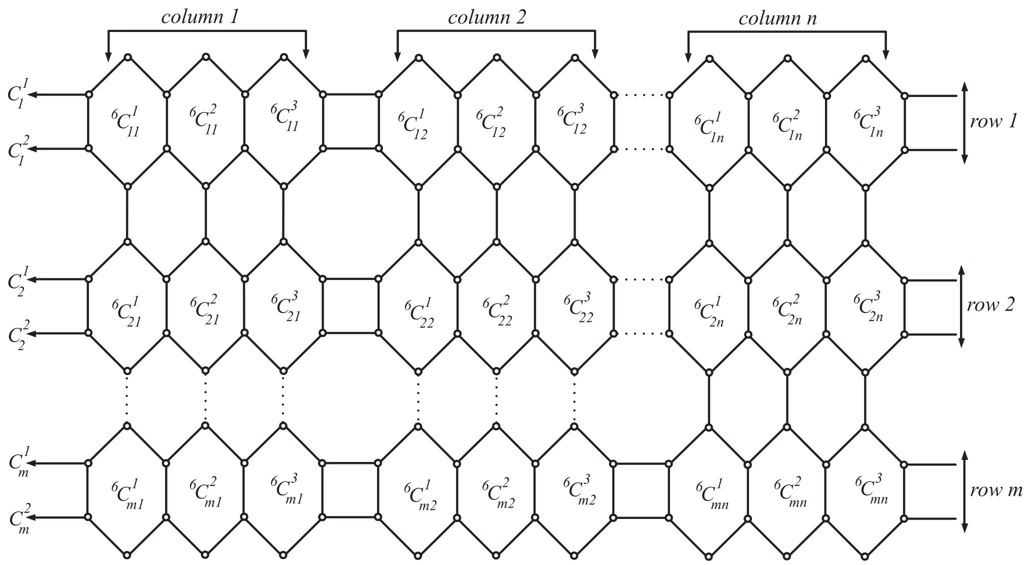

Figure 5. H-anthracenic nanotube.

Excessive index of H-anthracenic nanotube

In this section, we compute the excessive index for H-anthracenic nanotube. Anthracene is a solid polycyclic aromatic hydrocarbon of formula $C_{14}H_{10}$, consisting of three fused benzene rings. It is a component of coal tar. Anthracene is used in the production of the red dye alizarin and other dyes. The H-anthracenic nanotube is a sequence of C_6, C_6, C_6, C_4, C_6, C_6, C_6, $C_4, \ldots$ in first row and a sequence of C_6, C_6, C_8, C_6, C_6, $C_8, \ldots$ in other row. These nanotubes can be symbolized as $HANT[p, q]$ in which p is the number of triple hexagons in first row and q is the number of alternative hexagons in the column as described in Figure 5. The number of vertices of H-Anthracenic nanotube is $14pq$, and the edges are $21pq - 2q$.[8]

Theorem 5.1. *Let G be a H-Anthraceric HANT* $[m, n]$ *nanotube, then* $\chi'_e(G) = 6$.

Proof. By Lemma 1.4, $\chi'_e(G) \geq 6$. We now proceed to prove that the lower bound is sharp. **Case 1: *n*-odd**

Perfect matchings M_1, M_2, M_3, M_4, M_5 and M_6 are selected as follows:
Step 1: (Selection of edges in M_1)

a. From C_1^1, select the acute edges of column j, j odd and obtuse edges of column j, j even and from C_1^2, select the acute edges of column j, j even and obtuse edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of squares induced by column j and $j+1$, j odd, together with the vertical edge of column n, with one end incident at an obtuse edge of C_i^1 and the other end incident at an acute edge of $C_i^2, 1 \leq i \leq m$. See Figure 6.

Step 2: (Selection of edges in M_2)

a. From C_1^1, select the obtuse edges of column j, j odd and acute edges of column j, j even and from C_1^2, select the obtuse edges of column j, j even and acute edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.

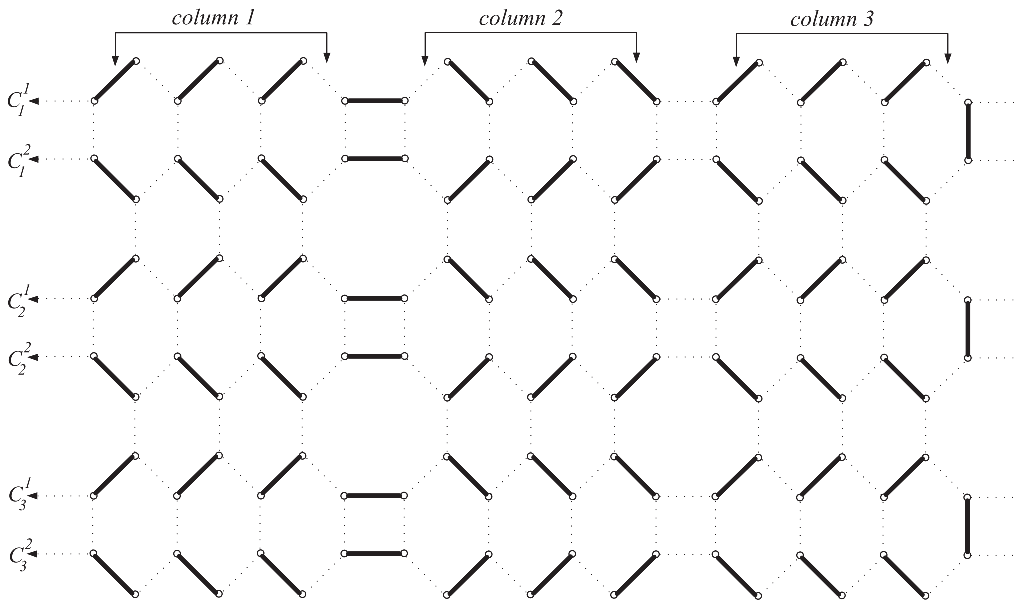

Figure 6. Selection of edges in M_1, when n is odd.

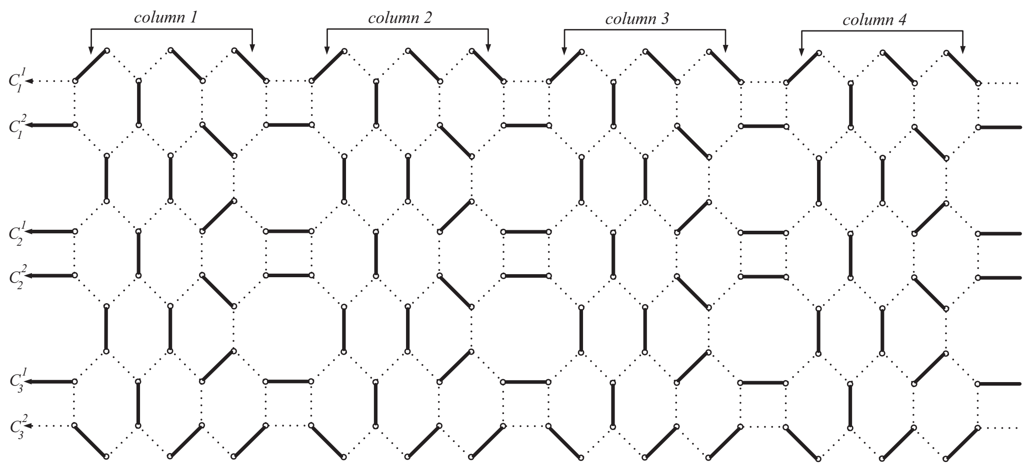

Figure 7. Selection of edges in M_3, when n is odd.

b. Select the horizontal edges of squares induced by column j and $j+1$, j-even, together with the vertical edges of column 1 with one end incident at an acute edge of C_i^1 and the other end incident at an obtuse edge of $C_i^2, 1 \leq i \leq m$. See Figure 7.

Step 3: (Selection of edges in M_3)

a. From C_1^1, select the acute and obtuse edges of ${}^6C_{11}^1$ and ${}^6C_{11}^2$ and from C_1^1 and C_1^2, select the obtuse edges of ${}^6C_{11}^3$. From C_i^1 and C_i^2, select the acute and obtuse edges of ${}^6C_{i1}^3, 1 < i < m$. From C_m^2, select the obtuse and acute edges of ${}^6C_{m1}^1$ and ${}^6C_{m1}^2$ and from C_m^1 and C_m^2, select the acute edges of ${}^6C_{m1}^3$. Repeat this process for all columns $j, 1 \leq j \leq n$.

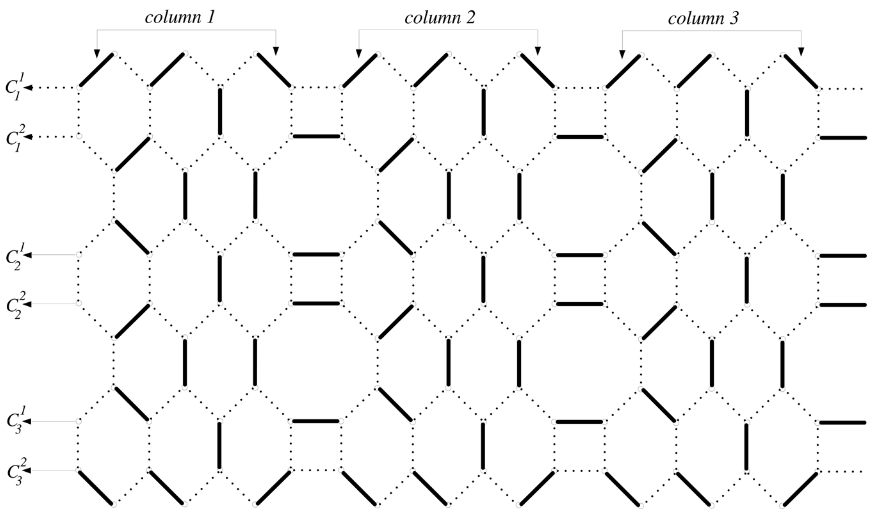

Figure 8. Selection of edges in M_4, when n is odd.

b. Select the common vertical edges between ${}^6C_{i1}^1$ and ${}^6C_{i1}^2, 1 \leq i \leq m$ and the vertical edges induced by ${}^6C_{i1}^1$ and ${}^6C_{(i+1)1}^1, {}^6C_{i1}^2$ and ${}^6C_{(i+1)1}^2, 1 \leq i < m$. Repeat this process for all columns $j, 1 \leq j \leq n$.
c. Select all the horizontal edges of squares induced by column j and $j+1,\ 1 \leq j \leq n$ except those horizontal edges of C_1^1 and C_m^2.

Step 4: (Selection of edges in M_4)

a. From C_1^1, select the acute and obtuse edges of ${}^6C_{11}^2$ and ${}^6C_{11}^3$ and from C_1^1 and C_1^2, select the acute edges of ${}^6C_{11}^1$. From C_i^1 and C_i^2, select the obtuse and acute edges of ${}^6C_{i1}^1,\ 1 < i < m$. From C_m^2, select the obtuse and acute edges of ${}^6C_{m1}^2$ and ${}^6C_{m1}^3$ and from C_m^1 and C_m^2, select the obtuse edges of ${}^6C_{m1}^1$. Repeat this process for all columns $j,\ 1 \leq j \leq n$.
b. Select the common vertical edge between ${}^6C_{i1}^2$ and ${}^6C_{i1}^3, 1 \leq i \leq m$ and the vertical edges induced by ${}^6C_{i1}^2$ and ${}^6C_{(i+1)1}^2, {}^6C_{i1}^3$ and ${}^6C_{(i+1)1}^3, 1 \leq i < m$. Repeat this process for all columns $j, 1 \leq j \leq n$.
c. Select all the horizontal edges of squares induced by column j and $j+1,\ 1 \leq j \leq n,$ except the horizontal edges of C_1^1 and C_m^2. See Figure 8.

Step 5: (Selection of edges in M_5)

a. From C_i^1, select the acute and from C_i^2, select the obtuse edges where $1 \leq i \leq m$ and for columns $j,\ 1 \leq j < n$. In column n, from C_i^1 select the obtuse edges and from C_i^2 select the acute edges for $1 \leq i \leq m$.
b. Select the both vertical edges of square induced by column $(n-1)$ and n together with the vertical edges of squares induced by column j and $j+1,\ 1 \leq j < n,$ with one end incident at an obtuse edges of C_i^1 and the other end incident at an acute edge of $C_i^2, 1 \leq i \leq m$. See Figure 9.

Step 6: (Selection of edges in M_6)

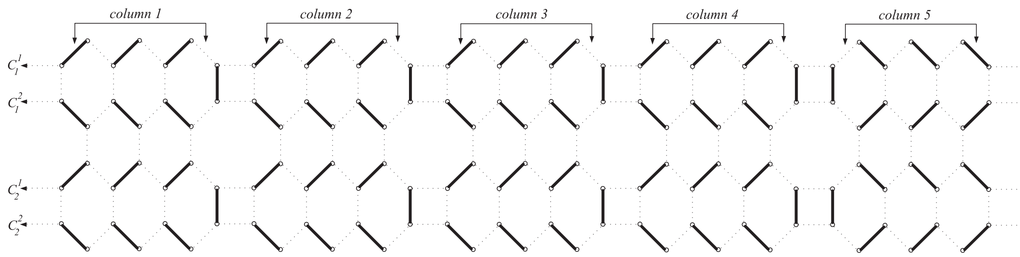

Figure 9. Selection of edges in M_5, when n is odd.

a. From C_i^1, select the obtuse edges and from C_i^2, select the acute edges where $1 \le i \le m$ and for columns $j, 1 \le j < n$. In column n, from C_i^1 select the acute edges from C_i^2 select the obtuse edges for $1 \le i \le m$.
b. Select both the horizontal edges of squares induced by column 1 and n, together with the vertical edges of squares induced by column j and $j+1$, $1 \le j < n$ with one end incident at an acute edge of C_i^1 and the other end incident at an obtuse edge of C_i^2, $1 \le i \le m$. See Figure 10.

Clearly the edges in M_1, M_2, M_3, M_4, M_5 and M_6 are selected in such a way that each $M_i, 1 \le i \le 6$ is perfect. Further, Steps 1(a) and 2(a) cover all acute and obtuse edges, Steps 1(b), 2(b), 3(c), 4(c), and 6(b) cover all horizontal edges and Steps 1(b), 2(b), 3(b), 4(b), 5(b), and 6(b) cover all vertical edges. Thus $\chi_e'(G) = 6$.

Case 2: n-even

Perfect matchings M_1, M_2, M_3, M_4, M_5 and M_6 are selected as follows:

Step 1: (Selection of edges in M_1)

a. From C_1^1, select the acute edges of column j, j odd and obtuse edges of column j, j even and from C_1^2 select the acute edges of column j, j even and obtuse edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \le i \le m$.
b. Select the horizontal edges of squares induced by column j and $j+1, j$ odd.

Step 2: (Selection of edges in M_2)

a. From C_1^1, select the obtuse edges of column j, j odd and acute edges of column j, j even and from C_1^2, select the obtuse edges of column j, j even and acute edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \le i \le m$.
b. Select the horizontal edges of squares induced by column j and $j+1$, j even together with both the vertical edges of squares induced by columns 1 and n.

Step 3:

The selection of edges in M_3, M_4, M_5 and M_6 are as in Case (1). See Figure 11. Clearly the edges in M_1, M_2, M_3, M_4, M_5 and M_6 are selected in such a way that each M_i, $1 \le i \le 6$ is perfect. Further, they cover all the acute, obtuse, horizontal and vertical edges of G. Thus, $\chi_e'(G) = 6$. □

Excessive index of *H*-tetracenic nanotube

In this section, we compute the excessive index for H-tetracenic nanotube. Tetracenic is the four ringed member of the series of acenes, it is also called 4-polyacenic. Let $G = G[p, q]$ be the H-tetracenic nanotube, with $18pq$ vertices. The H-tetracenic nanotubes is a sequence of C_6, C_6, C_6, C_6,

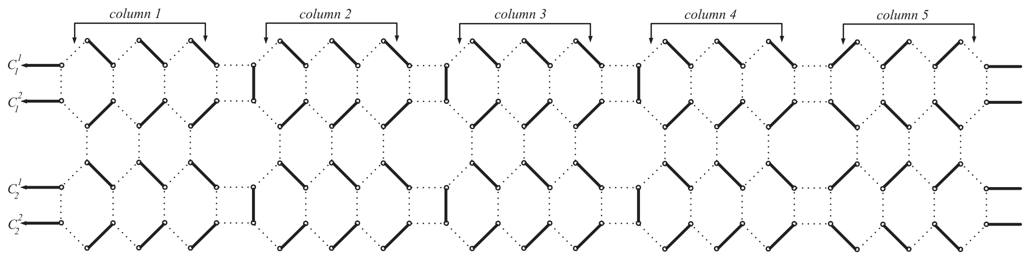

Figure 10. Selection of edges in M_6, when n is odd.

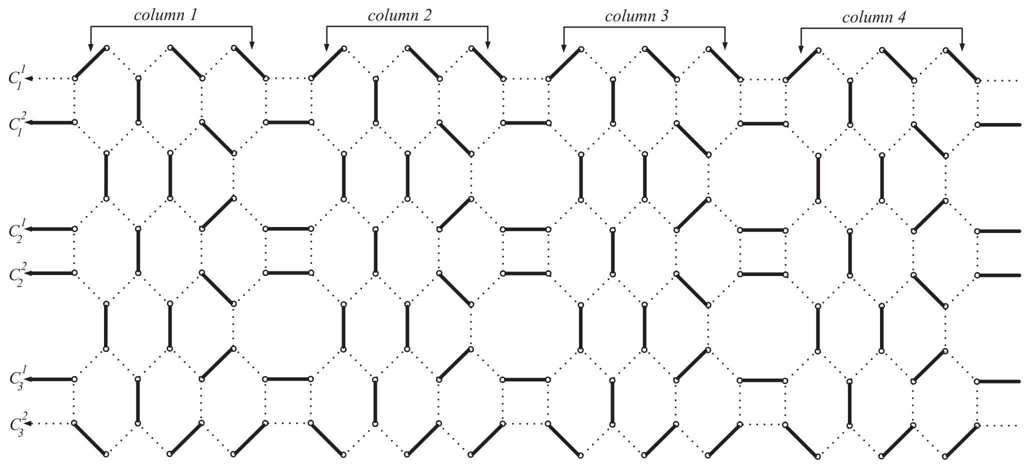

Figure 11. Selection of edges in M_3, when n is even.

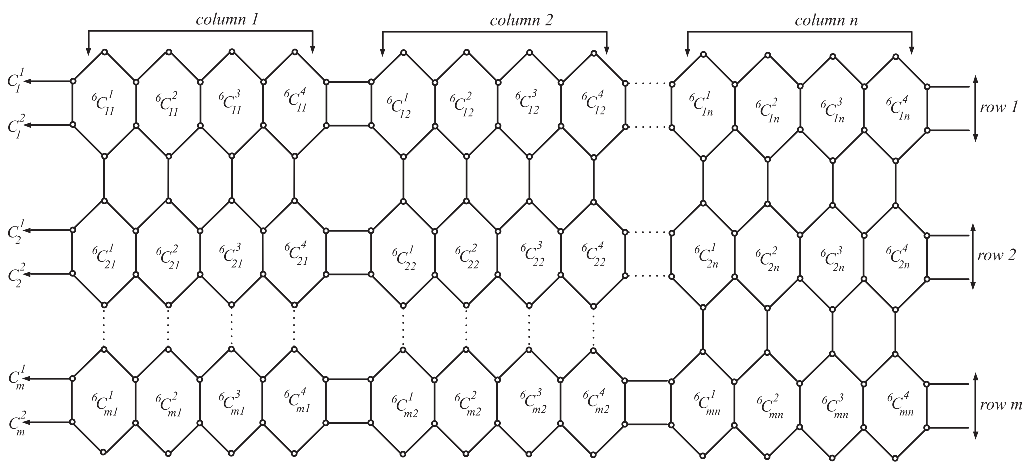

Figure 12. H-tetracenic nanotube.

C_4, C_6, C_6, C_6, C_6, C_4, ... in first row and a sequence of C_6, C_6, C_6, C_8, C_4, C_6, C_6, C_8, ... in other row.[8] See Figure 12.

Theorem 6.1. *Let G be a H-tetracenic nanotube* $[m, n]$. *Then* $\chi'_e(G) = 7$

Proof. By Lemma 1.4, $\chi'_e(G) \geq 7$. We now proceed to prove that the lower bound is sharp.

Case 1: ***n*-odd** Perfect matchings $M_1, M_2, M_3, M_4, M_5, M_6$ and M_7 are selected as follows.
Step 1: (Selection of edges in M_1)

a. From C_1^1, select the acute edges of column j, j odd and obtuse edges of column j, j even and from C_1^2, select the acute edges of column j, j even and obtuse edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of squares induced by column j and $j+1$, j odd, together with the vertical edge of column n, with one end incident at an obtuse edge of C_i^1 and the other end incident at an acute edge of $C_i^2, 1 \leq i \leq m$.

Step 2: (Selection of edges in M_2)

a. From C_1^1, select the obtuse edges of column j, j odd and acute edges of column j, j even and from C_1^2, select the obtuse edges of column j, j even and acute edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of squares induced by column j and $j+1$, j-even, together with the vertical edges of column 1 with one end incident at an acute edge of C_i^1 and the other end incident at an obtuse edge of $C_i^2, 1 \leq i \leq m$.

Step 3: (Selection of edges in M_3)

a. From C_1^1, select the acute edges of ${}^6C_{11}^1$ and the obtuse edges of ${}^6C_{11}^2$ and from C_1^1 and C_1^2, select the obtuse edges of ${}^6C_{11}^3$ and ${}^6C_{11}^4$. From C_i^1, select the acute edges of ${}^6C_{i1}^3$ and ${}^6C_{i1}^4, 1 < i < m$ and from C_i^2, select the obtuse edges of ${}^6C_{i1}^3$ and ${}^6C_{i1}^4, 1 < i < m$. From C_m^2, select the obtuse edges of ${}^6C_{m1}^1$ and the acute edge of ${}^6C_{m1}^2$ and from C_m^1 and C_m^2, select the acute edges of ${}^6C_{m1}^3$ and ${}^6C_{m1}^4$. Repeat the above processes for all column $j, 1 \leq j \leq n$.
b. Select the common vertical edges between ${}^6C_{i1}^1$ and ${}^6C_{i1}^2, 1 \leq i \leq m$ and the vertical edges induced by ${}^6C_{i1}^1$ and ${}^6C_{(i+1)1}^1, {}^6C_{i1}^2$ and ${}^6C_{(i+1)1}^2, 1 \leq i \leq m$. Repeat this process for all columns $j, 1 \leq j \leq n$.

(c) Select all the horizontal edges of squares induced by column j and $j+1,\ 1 \leq j \leq n,$ except those horizontal edges of C_1^1 and C_m^2.
Step 4: (Selection of edges in M_4)

a. From C_1^1, select the acute edges of ${}^6C_{11}^1$ and ${}^6C_{11}^2$ and select the obtuse edges of ${}^6C_{11}^3$ and ${}^6C_{11}^4$. From C_1^2 select the acute edges of ${}^6C_{11}^1$ and the obtuse edge of ${}^6C_{11}^4$. From C_i^1, select the obtuse edges of ${}^6C_{i1}^1$, and the acute edge of ${}^6C_{i1}^4, 1 < i \leq m$ and from C_i^2, select the acute edge of ${}^6C_{i1}^1$ and the obtuse edge of ${}^6C_{i1}^4, 1 < i < m$. From C_m^2, select the obtuse edges of ${}^6C_{m1}^1$ and ${}^6C_{m1}^2$ and the acute edges of ${}^6C_{m1}^3$ and ${}^6C_{m1}^4$. Repeat the above process for all columns $j,\ 1 \leq j \leq n$.
b. Select the common vertical edge between ${}^6C_{i1}^2$ and ${}^6C_{i1}^3, 1 \leq i \leq m$ and the vertical edges induced by ${}^6C_{i1}^2$ and ${}^6C_{(i+1)1}^2, {}^6C_{i1}^3$ and ${}^6C_{(i+1)1}^3, 1 \leq i < m$. Repeat this process for all columns $j, 1 \leq j \leq n$.(c) Select all the horizontal edges of squares induced by column j and $j+1$, $1 \leq j \leq n$, except those horizontal edges of C_1^1 and C_m^2.

Step 5: (Selection of edges in M_5)

a. From C_1^1, select the acute edges of ${}^6C_{11}^1, {}^6C_{11}^2$ and ${}^6C_{11}^3$ and from C_1^2, select the acute edges of ${}^6C_{11}^1$ and ${}^6C_{11}^2$. From C_i^1 select the obtuse edges of ${}^6C_{i1}^1$ and ${}^6C_{i1}^2, 1 < i \leq m$, and from C_i^2 select the acute edges of ${}^6C_{i1}^1, {}^6C_{i1}^2, 1 < i < m$. From C_m^2, select the obtuse edges of ${}^6C_{m1}^1, {}^6C_{m1}^2$ and ${}^6C_{m1}^3$ and the acute edge of ${}^6C_{m1}^4$. Repeat the above process for all columns $j, 1 \leq j \leq n$.
b. Select the common vertical edges between ${}^6C_{i1}^3$ and ${}^6C_{i1}^4, 1 \leq i \leq m$ and the vertical edges induced by ${}^6C_{i1}^3$ and ${}^6C_{(i+1)1}^3, {}^6C_{i1}^4$ and ${}^6C_{(i+1)1}^4, 1 \leq i < m$. Repeat this process for all columns $j,\ 1 \leq j \leq n$.

c. Select all the horizontal edges of squares induced by column j and $j+1$, $1 \leq j \leq n$, except those horizontal edges of C_1^1 and C_m^2

Step 6: (Selection of edges in M_6)

a. From C_i^1, select the acute edges and from C_i^2, select the obtuse edges where $1 \leq i \leq m$ and for columns $j, 1 \leq j < n$. In column n, from C_i^1 select the obtuse edges from C_i^2 select the acute edges for $1 \leq i \leq m$.
b. Select both the vertical edges of squares induced by column $n - 1$ and n, together with the vertical edges of squares induced by column j and $j+1$, $1 \leq j < n$ with one end incident at an obtuse edge of C_i^1 and the other end incident at an acute edge of C_i^2, $1 \leq i \leq m$.

Step 7: (Selection of edges in M_7)

a. From C_i^1, select the obtuse edges and from C_i^2, select the acute edges where $1 \leq i \leq m$ and for columns $j, 1 \leq j < n$. In column n, from C_i^1 select the acute edges and from C_i^2 select the obtuse edges for $1 \leq i \leq m$.
b. Select both the horizontal edges of squares induced by columns 1 and n, together with the vertical edges of squares induced by columns j and $j+1, 1 \leq j < n$ with one end incident and an acute edge of C_i^1 and the other end incident at an obtuse edge of $C_i^2, 1 \leq i \leq m$.

Clearly the edges in $M_1, M_2, M_3, M_4, M_5, M_6$ and M_7 are selected in such a way that each $M_i, 1 \leq i \leq 7$ is perfect. Further, Steps 1(a) and 2(a) cover all acute and obtuse edges, Steps 1(b), 2(b), 3(c), 4(c), 5(c), and 7(b) cover all horizontal edges and Steps 1(b), 2(b), 3(b), 4(b), 5(b), 6(b), and 7(b) cover all vertical edges. Thus $\chi'_e(G) = 7$.
Case 2: n-even

Perfect matchings $M_1, M_2, M_3, M_4, M_5, M_6$ and M_7 are selected as follows:
Step 1: (Selection of edges in M_1)

a. From C_1^1, select the acute edges of column j, j odd and obtuse edges of column j, j even and from C_1^2, select the acute edges of column j, j even and obtuse edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of squares induced by column j and $j+1, j$ odd.

Step 2: (Selection of edges in M_2)

a. From C_1^1, select the obtuse edges of column j, j odd and acute edges of column j, j even and from C_1^2, select the obtuse edges of column j, j even and acute edges of column j, j odd. Repeat this process for all C_i^1 and $C_i^2, 1 \leq i \leq m$.
b. Select the horizontal edges of squares induced by column j and $j+1$, j even together with both the vertical edges of squares induced by columns 1 and n. The edges in M_3, M_4, M_5, M_6 and M_7 are selected as in Case (1). Clearly the edges in $M_1, M_2, M_3, M_4, M_5, M_6$ and M_7 are selected in such a way that each M_i, $1 \leq i \leq 7$ is perfect. Further, $M_i, 1 \leq i \leq 7$, cover all the acute, obtuse, horizontal and vertical edges of G. Thus, $\chi'_e(G) = 7$. □

Conclusion

In this article, we determined the excessive index for $TUC_4C_8(S)[p,q]$ nanosheet, $NPHX[m,n]$ nanotube, $TUC_4C_8(R)[p,q]$ nanotube, H-anthracenic nanotube and H-tetracenic nanotube. It would be an interesting line of research to determine the excessive index for other chemical structures since scheduling theory has gained momentum in biotechnology and even in nanotechnology.

Disclosure statement

No potential conflict of interest was reported by the authors.

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