The locating-chromatic number and partition dimension of fibonacene graphs

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Abstract

Fibonacenes are unbranched catacondensed benzenoid hydrocarbons in which all the non-terminal hexagons are angularly annelated. A hexagon is said to be angularly annelated if the hexagon is adjacent to exactly two other hexagons and possesses two adjacent vertices of degree 2. Fibonacenes possess remarkable properties related with Fibonacci numbers. Various graph properties of fibonacenes have been extensively studied, such as their saturation numbers, independence numbers and Wiener indices.

In this paper, we show that the locating-chromatic number of any fibonacene graph is 4 and the partition dimension of such a graph is 3.

1. Introduction

Many applications of graphs can be found in chemistry. Chemical graphs were first introduced in the middle of the 18th century. Graph theory is increasingly popular in chemistry because almost all problems in chemistry can be modeled in simple graphs that directly represent molecules, chemical bonds and so on. Furthermore, graph theory provides simple rules so that it can obtain many qualitative predictions about the structure and reactivity of various compounds. Seeing the benefits of graph theory in chemistry, this is interesting to discuss.

Gutman dan Klav$\check{z}$ar [12] discussed the chemical graph theory of fibonacenes. A *benzenoid system* is a connected plane graph without cut-vertices in which all inner faces are hexagons, such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge. A benzenoid system is said to be *unbranched catacondensed* if it does not possess a vertex shared by three hexagons and not possess a hexagon having three neighboring hexagons. *Fibonacenes* are unbranched catacondensed benzenoid hydrocarbons in which all the non-terminal hexagons are angularly annelated. A hexagon is said to be *angularly annelated* if the hexagon is adjacent to exactly two other hexagons and possesses two adjacent vertices of degree 2. Previously fibonacenes were introduced by Balaban [5], although it seems to be first mentioned by Anderson [2]. Fibonacenes have the Kekul$\acute{e}$ structure, which is in graph theory it is called a perfect matching. The number of perfect matching from fibonacenes with h hexagon forms Fibonacci numbers. Balaban [5] gives the name fibonaccene. However, he suppressed one c for simplicity and for similarity with the established name "acenes".

There are several papers that have discussed benzenoid specifically fibonacenes, such as Wiener index [9], saturation number [10], and independence number [15]. The applications of these topics in chemistry have also been mentioned in [9, 10, 15].

The concept of the locating-chromatic number was first introduced by Chartrand et al. [6]. The locating-chromatic number concept of a graph is as a combination of two concepts that is the graph coloring concept and the partition dimension concept. The concept of the partition dimension of a graph was introduced by Chartrand et al. [7] as an extension of the metric dimension concept introduced by Harary and Melter [13].

In this paper, we consider only simple connected graphs. Let $G(V, E)$ be a graph with the vertex-set V and edge-set E. For a vertex v of a connected graph G and a subset S of $V(G)$, the *distance* between v and S is $d(v, S) = \min\{d(v, x) \mid x \in S\}$. Let $N(v)$ be the set of vertices adjacent to v. For an ordered $k-$partition $\Pi = \{S_1, S_2, \ldots, S_k\}$ of $V(G)$, the *representation* of v with respect to Π is the ordered k-tuple $r(v \mid \Pi) = (d(v, S_1), d(v, S_2), \ldots, d(v, S_k))$. The k-partition Π is a *resolving partition* if the ordered k-tuple $r(v \mid \Pi), v \in V(G)$, are distinct. The minimum k for which there is a resolving k-partition of $V(G)$ is the *partition dimension* $pd(G)$ of G.

Chartrand et al [8] characterized all graphs with partition dimension 2, and all graphs on n vertices with partition dimension $n - 1$ or n. Lately, Tomescu [19] characterized all graph of order n having partition dimension $n - 2$.

Proposition 1.1. *[8] A connected graph G has partition dimension 2 if and only if G is a path.*

The following lemma appeared in [8] will be useful to us.

Lemma 1.1. *[8] Let Π be a resolving partition of $V(G)$ and $u, v \in V(G)$. If $d(u, w) = d(v, w)$ for all $w \in V(G)\backslash\{u, v\}$ then u and v belong to distinct element of Π.*

Next, let $G(V, E)$ be a graph with the vertex-set V and edge-set E. Let c be a proper coloring of G, namely $c(u) \neq c(v)$ for any adjacent vertices u and v in G. Let c be a k-coloring of G and $\Pi = \{C_1, C_2, \ldots, C_k\}$ be a partition of $V(G)$ induced by c, where C_i is the set of vertices receiving color i for $1 \leq i \leq k$. The *color code* $c_\Pi(v)$ of v is defined as the ordered k-tuple

$(d(v, C_1), d(v, C_2), \ldots, d(v, C_k))$. If all vertices of G have distinct color codes, then c is called a *locating-chromatic k-coloring* of G (*k-locating coloring*, in short). *The locating-chromatic number* of a graph G, denoted by $\chi_L(G)$, is the smallest k such that graph G admits a $k-$locating coloring.

The following theorem taken from paper of Chartrand et al. [6] is a fundamental theorem about the locating chromatic number of a graph.

Theorem 1.1. *[6] Let c be a locating coloring in a connected graph G. If u and v are distinct vertices of G such that $d(u, w) = d(v, w)$ for all $w \in V(G) \backslash \{u, v\}$, then $c(u) \neq c(v)$. In particular, if u and v are non-adjacent vertices of G such that $N(u) = N(v)$, then $c(u) \neq c(v)$.*

Theorem 1.2. *[6] The locating chromatic number of a cycle C_n is 3 for odd n and 4 for otherwise.*

Many papers studied about the partition dimension that containing cycles, see [18, 14, 1]. While, various results of the locating-chromatic number that containing cycles, see [16, 17, 4, 11]. In [3], Asmiati and Baskoro characterized all graph containing cycles with locating-chromatic number three.

In this paper, we show that the locating-chromatic number and the partition dimension of fibonacene graphs are 4 and 3, respectively.

2. Main Results

For $h \geq 1$, let $F(h)$ be any fibonacene graph. Then, $F(h)$ has $n = 4h + 2$ vertices of which $2h + 4$ are of degree 2 and $2h - 2$ of degree 3. The $F(h)$ may have type as helicene (H_h), zig-zag fibonacene (Z_h), serpent (S_h), and any combination of them depicted in Figure 1.
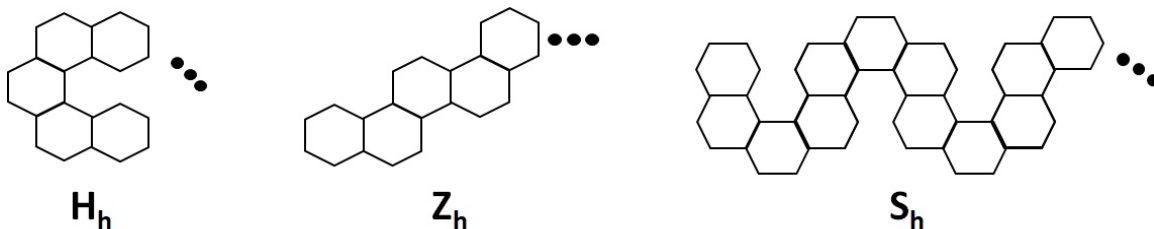

Figure 1. Three extremal fibonacenes.

2.1. Locating-chromatic number of fibonacene graphs

This subsection will present the result of the locating-chromatic number for graph $F(h)$.

Theorem 2.1. *Let $F(h)$ be a connected fibonacene graph with h hexagons, then $\chi_L(F(h)) = 4$.*

Proof. Let $V(F(h)) = \{v_0, v_1, v_2, \ldots, v_{n-1}\}$ where v_0 is a fixed vertex of degree 2 in terminal hexagon and $v_0, v_1, v_2, \ldots, v_{n-1}$ are cyclicly ordered by Hamiltonian. Let $E(F(h)) = \{v_i v_{i+1} \mid i = 0, 1, \ldots, n - 2\} \cup \{v_0 v_{n-1}\} \cup I$, where I is the set of internal edges between two adjacent hexagons. For a contrary suppose $\chi_L(F(h)) \leq 3$. Since $F(h)$ is not a path then $\chi_L(F(h)) > 2$. Now, let c be a $3-$coloring on $F(h)$ where $C_i = \{v \in V(F(h)) \mid c(v) = i\}$.

1. There exists one hexagon with 2 colors. let H be the hexagon with 2 colors (1 and 2). Now, consider the vertex u with the third color and with minimum distance to hexagon H. Without loss of generality, we may assume the vertex u is in the right side of hexagon H, depicted in Figure 2. Assume the distance from u to H is equal to $d(u, v_i)$. Then, the color codes of the two neighbors of v_i in H are the same, namely $(1, 0, d(u, v_i) + 1)$.
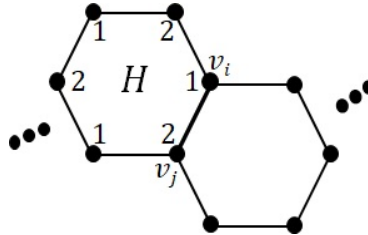

Figure 2. Fibonacene graph coloring with there exists one hexagon with 2 colors.

2. At least one hexagon contains 3 colors.
   There are three cases to be considered as depicted in Figure 3. In each case, there are two vertices with the same color codes. These color codes are shown in bold.
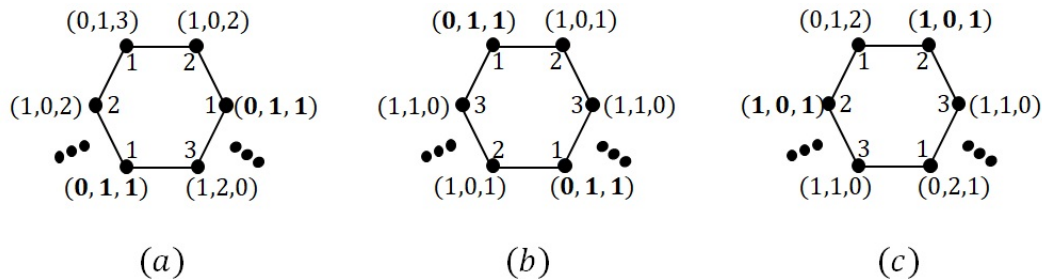

Figure 3. Fibonacene graph coloring with at least one hexagon contains 3 colors.

Therefore, $\chi_L(F(h)) \geq 4$.

Next, define $A_i(v_0) = \{v \in F(h) \mid d(v, v_0) = i\}$ for $i \in [0, d_{max}]$ where $d_{max} = \max\{d(v, v_0)\}$. For any i, we have that $|A_i(v_0)| \leq 4$ since the distribution of all vertices at distance i from v_0 can be depicted in Figure 4.
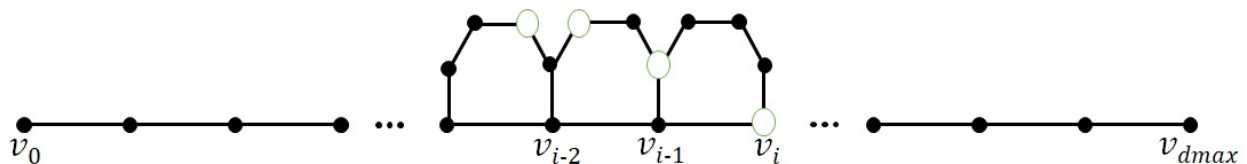

Figure 4. The shortest path from v_0 to $v_{d_{max}}$.

Now, define a coloring in $F(h)$ by using algorithm 1.

Algorithm 1 (Finding locating coloring in fibonacene graph).

Let $c : V(F(h)) \rightarrow \{1, 2, 3, 4\}$ such that :

1. $c(v_0) = 1$.
2. For $i = 1$ to i_{max} do the following actions.

Case 1. $|A_i(v_0)| = 2$ or $|A_i(v_0)| = 3$. Define $c(A_i(v_0)) \rightarrow \{2, 3, 4\}$ such that $|c(A_i(v_0))| = |A_i(v_0)|$ and we always use the smallest possible colors in the following ordering.

    1. Color a vertex v (if any) in $A_i(v_0)$ where $|N(v) \cap A_{i-1}(v_0)| = 2$.
    2. Color at most two vertices v and w in $A_i(v_0)$ where $|N(v) \cap N(w) \cap A_{i-1}(v_0)| = 1$.
    3. Color a vertex v in $A_i(v_0)$ where $|N(v) \cap A_{i-1}(v_0)| = 1$.

Case 2. $|A_i(v_0)| = 4$. Let $A_i(v_0) = \{a_1, a_2, a_3, a_4\}$. Now define a coloring $c(A_i(v_0)) \rightarrow \{2, 3, 4\}$ such that we always use the smallest possible colors in the following ordering.

    1. Color vertex a_1 in $A_i(v_0)$ where $|N(a_1) \cap A_{i-1}(v_0)| = 2$.
    2. Color vertex a_2 in $A_i(v_0)$ and $c(a_2) = c(a_1)$, where $|N(a_1) \cap N(a_2) \cap A_{i-1}(v_0)| = 1$.
    3. Color a vertex $v \in A_{i+1}(v_0)$ with $v \in N(a_2)$ such that $c(v) = c(s)$ where $s \in N(a_1) \cap N(a_2) \cap A_{i-1}(v_0)$.
    4. Color vertex a_3 where $a_3 \in N(v) \cap A_i(v_0)$.
    5. Color the remaining vertex in $A_i(v_0)$.

end algorithm 1.

We will show that c is a locating-coloring on $F(h)$. To do so, we have to prove that for any two vertices x and y in $F(h)$, their color codes are distinct. Let $\Pi = \{C_1, C_2, C_3, C_4\}$ be the partition of $V(F(h))$ induced by the above coloring c with $C_i = \{v \in F(h) \mid c(v) = i\}$. Take any two vertices x and y in $F(h)$ such that $c(x) = c(y)$. Of course $x \neq v_0$ and $y \neq v_0$. If $d(x, v_0) \neq d(y, v_0)$ then $c_\Pi(x) \neq c_\Pi(y)$. Now, if $d(x, v_0) = d(y, v_0)$ then $x, y \in A_i(v_0)$ for some i and $|A_i(v_0)| = 4$. So $c_\Pi(x) \neq c_\Pi(y)$ because $d(x, C_j) = 1$ and $d(y, C_j) = 2$ for some $j \in \{2, 3, 4\}$.

Therefore, c is a locating-coloring on $F(h)$ and $\chi_L(F(h)) = 4$. $\qquad\square$

For $h \geq 1$, let $G(h)$ be any unbranched catacondensed benzenoid graph. In this case, $G(h)$ can have linearly annelated hexagons as depicted in Figure 5. A hexagon is said to be linearly annelated if it is adjacent to exactly two other hexagons and it does not have two adjacent vertices of degree 2. Therefore, any graph $G(h)$ can be a fibonacene or not.

Theorem 2.2. *Let $G(h)$ be a connected unbranched catacondensed benzenoid graph with h hexagons, then $\chi_L(G(h)) = 4$.*

Proof. The proof is the same as the one of Theorem 2.1, since the method used in Theorem 2.1 can be also applied to the graph that contains linearly annelated hexagons. $\qquad\square$
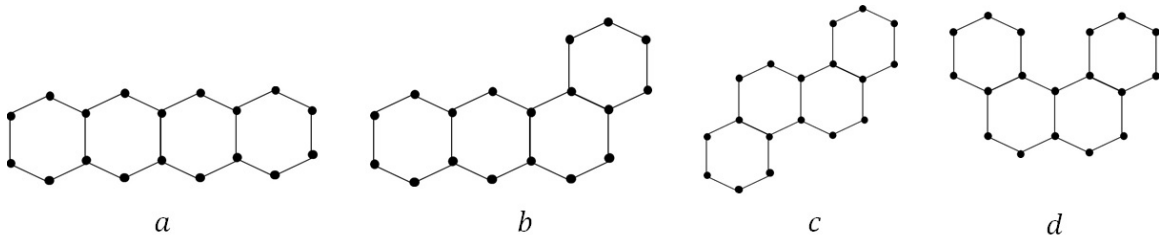
Figure 5. Unbranched catacondensed benzenoid graphs with 4 hexagons. The graphs in (c) and (d) are fibonacenes and the graphs in (a) and (b) contain linearly annelated hexagons.

2.1.1. Partition dimension of fibonacene graphs

This subsection will present the result of the partition dimension for fibonacene graphs.

Theorem 2.3. *Let $F(h)$ be a connected fibonacene graph with h hexagons, then $pd(F(h)) = 3$.*

Proof. Let $V(F(h)) = \{v_0, v_1, v_2, \ldots, v_{n-1}\}$ where v_0 is a fixed vertex of degree 2 in terminal hexagon and $v_0, v_1, v_2, \ldots, v_{n-1}$ are cyclically ordered by Hamiltonian. Let $E(F(h)) = \{v_i v_{i+1} \mid i = 0, 1, \ldots, n-2\} \cup \{v_0 v_{n-1}\} \cup I$, where I is the set of internal edges between two adjacent hexagons. According to Proposition 1.1, $pd(F(h)) \geq 3$. For $i \in [0, d_{max}]$ where $d_{max} = \max \{d(v, v_0)\}$, define $A_i(v_0) = \{v \in (F(h)) \mid d(v, v_0) = i\}$. Since the distribution of all vertices at distance i from v_0 can be depicted in Figure 4, then $|A_i(v_0)| \leq 4$ for any i.

Next, let $\Pi_1 = \{S_1, S_2, S_3\}$ be a partition on $V(F(h))$ induced by a mapping $l : V(F(h)) \longrightarrow \{1, 2, 3\}$ by using the following algorithm.

Algorithm 2 (Finding resolving partition in fibonacene graph.)
Partition all vertices in $V(F(h))$ by following steps.

1. Define $l(v_0) = 1$ and $l(v_{d_{max}}) = 2$.
2. For $i = 1$ to $d_{max} - 1$ do

Case 1 $|A_i(v_0)| = 2$ and let $A_i(v_0) = \{a_1, a_2\}$. Then, assign $l(a_1) = 2$ and $l(a_2) = 3$ if $|N(a_1) \cap A_{i-1}(v_0)| \geq |N(a_2) \cap A_{i-1}(v_0)|$.

Case 2 $|A_i(v_0)| = 3$ and let $A_i(v_0) = \{a_1, a_2, a_3\}$. Then, these three vertices a_1, a_2, a_3 must be located in two neighboring hexagons. Let a_1 be the vertex contained in the closest hexagon to terminal hexagon that contains v_0. Now choose a_3 such that $N(a_1) \cap N(a_3) \notin A_{i-1}(v_0) \cup A_{i+1}(v_0)$.

    1. If $|A_{i-1}(v_0)| = 2$ or $|A_{i-1}(v_0)| = 3$, then $l(a_1) = l(a_3) = 2$ and $l(a_2) = 3$.

    2. If $|A_{i-1}(v_0)| = 4$ and let k be the smallest nonnegative integer such that $|A_{i-2-k}| = 3$, then assign

$$(l(a_1), l(a_2), l(a_3)) = \begin{cases} (3, 3, 2), & \text{if } k \equiv 0 \pmod 4 \\ (2, 3, 2), & \text{if } k \equiv 1 \pmod 4 \\ (2, 2, 3), & \text{if } k \equiv 2 \pmod 4 \\ (2, 3, 2), & \text{if } k \equiv 3 \pmod 4. \end{cases}$$

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Case 3 $|A_i(v_0)| = 4$ and let $A_i(v_0) = \{a_1, a_2, a_3, a_4\}$. Then, these four vertices a_1, a_2, a_3, a_4 must be located in three hexagons consequtively. Let a_1 be the vertex contained in the closest hexagon to terminal hexagon that contains v_0 and choose a_2 such that $N(a_1) \cap N(a_2) \in A_{i-1}(v_0)$. Let a_4 be the vertex contained in the farthest hexagon to terminal hexagon that contains v_0 and choose a_3 such that $N(a_3) \cap N(a_4) \in A_{i-1}(v_0)$. Moreover $N(a_2) \cap N(a_3) \in A_{i+1}(v_0)$. Let k be the smallest nonnegative integer such that $|A_{i-2-k}| = 3$, then assign

$$(l(a_1), l(a_2), l(a_3), l(a_4)) = \begin{cases} (2,3,3,2), & \text{if } k \equiv 0 \pmod 4 \\ (3,3,2,2), & \text{if } k \equiv 1 \pmod 4 \\ (2,2,2,3), & \text{if } k \equiv 2 \pmod 4 \\ (2,2,3,2), & \text{if } k \equiv 3 \pmod 4. \end{cases}$$

end algorithm 2.

We will show that l is a resolving partition on $F(h)$. To do so, we have to show that for any two vertices x and y, their repsensations will be sdistinct. Take any two vertices x and y in $F(h)$ such that $l(x) = l(y)$. Of course, $x \neq v_0$ and $y \neq v_0$. If $d(x, v_0) \neq d(y, v_0)$ then $r(x|\Pi_1) \neq r(y|\Pi_1)$. Now, if $d(x, v_0) = d(y, v_0)$ then we have $x, y \in A_i(v_0)$ for some i. Note that the symbol $(a; b; \ldots, c)$ represents $|A_{i-1}(v_0)| = a$, $|A_i(v_0)| = b$ and $|A_{i+k}(v_0)| = c$ for some k.

1. If $|A_i(v_0)| = 3$ then the only possible distribution of the vertices at distance $i - 1$, i and $i + 1$ from v_0 are $(2; 3; 3)$, $(2; 3; 4)$, $(3; 3; 1)$, $(3; 3; 2)$, $(4; 3; 1)$, $(4; 3; 2)$. For the first four cases namely $(2; 3; 3)$, $(2; 3; 4)$, $(3; 3; 1)$, and $(3; 3; 2)$, all vertices in $A_{i-1}(v_0)$, $A_i(v_0)$ and $A_{i+1}(v_0)$ will be partitioned according to Algorithm 2. Therefore, we have $l(a_1) = l(a_3) = 2$ and $l(a_2) = 3$ so $x = a_1$ and $y = a_3$. In these case, we have that $r(x|\Pi_1) \neq r(y|\Pi_1)$, as shown in Figure 6. All vertices in $A_{i-1}(v_0)$, $A_i(v_0)$, $A_{i+1}(v_0)$ respectively is indicated by $\square$, $\circ$, $\triangle$. For the cases of $(4; 3; 1)$ and $(4; 3; 2)$, we will discuss later in case of $|A_i(v_0)| = 4$.

2. If $|A_i(v_0)| = 4$ then the only possible distribution of vertices at distance $i - 1$, i and $i + 1$ from v_0 are $(3; 4; 3)$, $(3; 4; 4)$, $(4; 4; 3)$, $(4; 4; 4)$. All four cases will be combined with cases of $(4; 3; 1)$ and $(4; 3; 2)$. If hexagon H is terminal hexagon then it will get the case of $(4; 3; 1)$. If hexagon H is not terminal hexagon then there are two possibilities for the addition of hexagon to keep forming a fibonacene graph. If e_2 is the internal edge then the next image will be obtained. If e_1 is the internal edge then it will get the case of $(4; 3; 2)$. Therefore, vertices x and y will be contained in $\circ$, $\triangle$, $\triangledown$, $\square$, $\triangleright$, and $\triangleleft$. All vertices in $A(v_0)$ will be partitioned according to cases 2.2 and 3 Algorithm 2. So, if $x, y \in A_i(v_0)$ for some i then $r(x|\Pi_1) \neq r(y|\Pi_1)$, as shown in Figure 7 and the representations of vertices can see on table 1.

Therefore, since for each vertices on $F(h)$ have distinct representations so $pd(F(h)) \leq 3$. We get $pd(F(h)) = 3$.
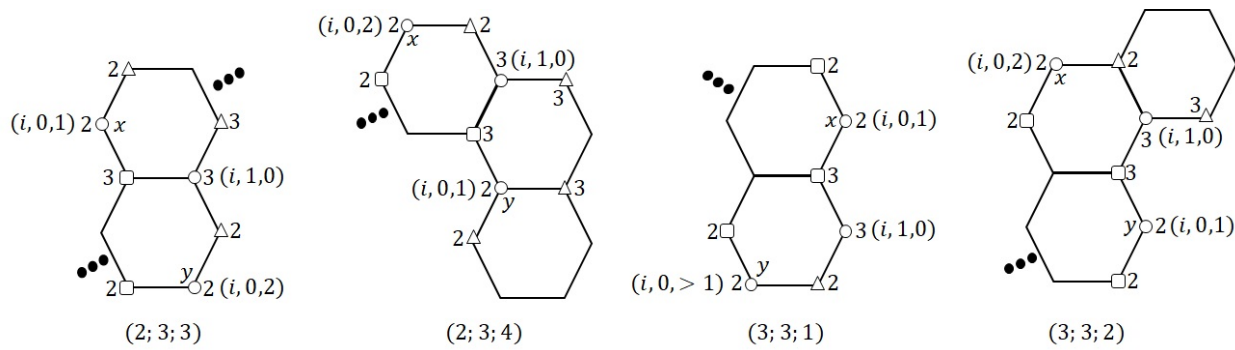
$\square$

Figure 6. The representations of vertices in $|A_i(v_0)| = 3$ for the cases of $(2;3;3)$, $(2;3;4)$, $(3;3;1)$, $(3;3;2)$.

3. Acknowledgement

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(a) $3; 4; 3; 1(2)$

(b) $3; 4; 4; 3; 1(2)$

(c) $3; 4; 4; 4; 3; 1(2)$

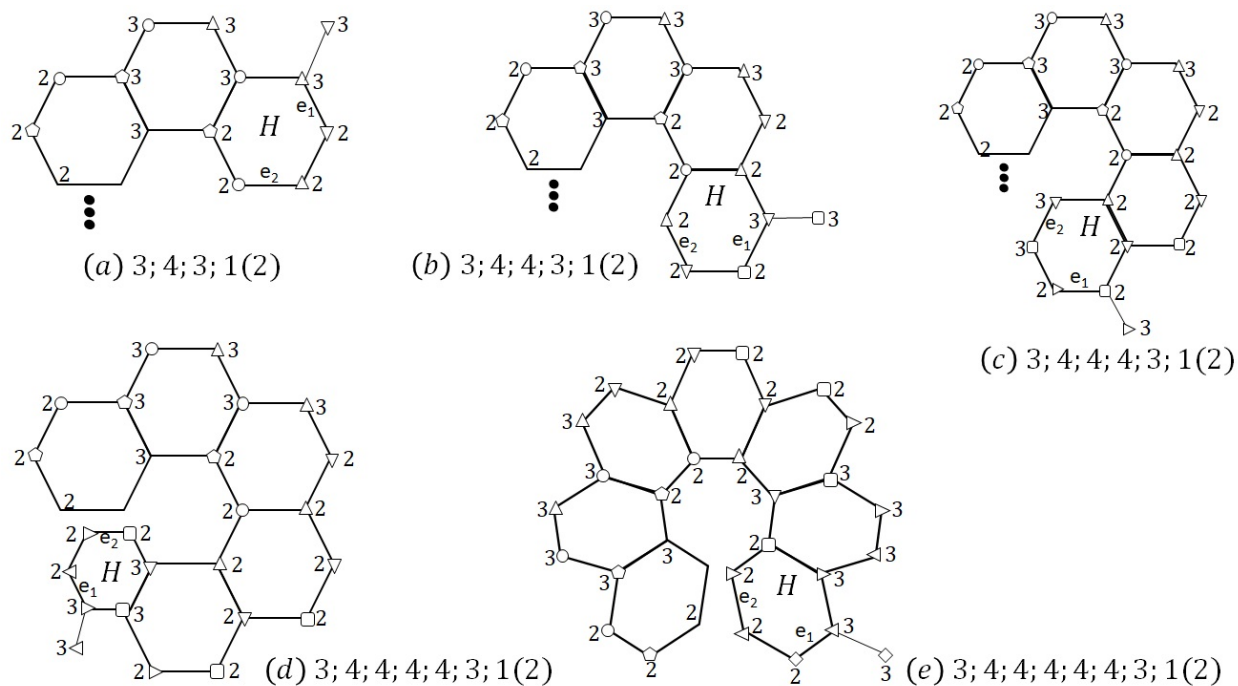(d) $3; 4; 4; 4; 4; 3; 1(2)$

(e) $3; 4; 4; 4; 4; 4; 3; 1(2)$

Figure 7. The cases of $|A_i(v_0)| = 4$.

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Table 1. Representations of vertices on some cases with $|A_i(v_0)| = 4$ and the cases of $(4;3;1)$ and $(4;3;2)$.

-	a	b	c	d	e
○	$(i,0,1)$ $(i,2,0)$ $(i,1,0)$ $(i,0,2)$	$(i,0,1)$ $(i,2,0)$ $(i,1,0)$ $(i,0,2)$	$(i,0,1)$ $(i,2,0)$ $(i,1,0)$ $(i,0,2)$	$(i,0,1)$ $(i,2,0)$ $(i,1,0)$ $(i,0,2)$	$(i,0,1)$ $(i,2,0)$ $(i,1,0)$ $(i,0,2)$
△	$(i+1,2,0)$ $(i+1,1,0)$ $(i+1,0,2)$ $-$	$(i+1,2,0)$ $(i+1,1,0)$ $(i+1,0,1)$ $(i+1,0,3)$	$(i+1,2,0)$ $(i+1,1,0)$ $(i+1,0,2)$ $(i+1,0,1)$	$(i+1,2,0)$ $(i+1,1,0)$ $(i+1,0,2)$ $(i+1,0,1)$	$(i+1,2,0)$ $(i+1,1,0)$ $(i+1,0,2)$ $(i+1,0,1)$
▽	$-$ $-$ $-$ $-$	$(i+2,0,1)$ $(i+2,1,0)$ $(i+2,0,2)$ $-$	$(i+2,0,1)$ $(i+2,0,3)$ $(i+2,0,2)$ $(i+2,1,0)$	$(i+2,0,1)$ $(i+2,0,3)$ $(i+2,0,2)$ $(i+2,1,0)$	$(i+2,0,1)$ $(i+2,0,3)$ $(i+2,0,2)$ $(i+2,1,0)$
□	$-$ $-$ $-$ $-$	$-$ $-$ $-$ $-$	$(i+3,0,3)$ $(i+3,0,2(1))$ $(i+3,1,0)$ $-$	$(i+3,0,3)$ $(i+3,0,2)$ $(i+3,1,0)$ $(i+3,0,1)$	$(i+3,0,3)$ $(i+3,0,2)$ $(i+3,1,0)$ $(i+3,0,1)$
▷	$-$ $-$ $-$ $-$	$-$ $-$ $-$ $-$	$-$ $-$ $-$ $-$	$(i+4,0,1)$ $(i+4,1,0)$ $(i+4,0,2)$ $-$	$(i+4,0,1)$ $(i+4,2,0)$ $(i+4,1,0)$ $(i+4,0,2)$
◁	$-$ $-$ $-$ $-$	$-$ $-$ $-$ $-$	$-$ $-$ $-$ $-$	$-$ $-$ $-$ $-$	$(i+5,2,0)$ $(i+5,1,0)$ $(i+5,0,2)$ $-$

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