On the minimum number of bond-edge types and tile types: an approach by edge-colorings of graphs

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Abstract

The purpose of this paper is twofold. On one hand, we want to describe from a new graph theory perspective the self-assembly of DNA structures with branched junction molecules having flexible arms. On the other hand, we employ edge-colorings and graph decompositions to study the well-known problem of determining the minimum number of bond-edge types and tile types, which are graph invariants appearing in this context. We provide a strategy that can be applied to arbitrary graphs for obtaining upper bounds for these graph invariants.

Keywords: DNA self-assembly strategy, bond-edge type, tile type, generalized chromatic index, palette index, graph decomposition.
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1 Introduction.

This paper deals with a graph theory problem related to the self-assembly of DNA structures. These constructs may have applications which include molecular scaffolding and drug delivery [16, 18, 21].

Several techniques that are based on the Watson-Crick complementary properties of DNA strands have been developed in order to obtain the self-assembly. For instance, the origami method [17], the brick method [13, 14] as well as flexible and rigid tiling [8, 10]. Here, we consider the method based on *branched junction molecules* (with flexible arms) [18], which are "star-like" molecules formed by several arms of DNA flanking a branch point. Each arm is, in the simplest case, a double strand of DNA where one strand extends further than the other and forms an adhesion site at the end of the arm called a *cohesive-end*. Each cohesive-end is an unsatisfied sequence of

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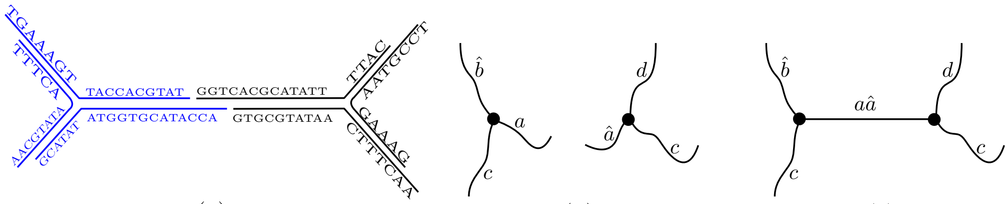
nitrogenous bases (A's, T's, C's, G's) and branched junction molecules having arms with complementary cohesive-ends can join together and form a larger complex. Following [3, 12], we assume that the arms of the molecules are flexible, so that all arms are allowed to move in any direction and all complementary cohesive-ends can bond together. Branched junction molecules with rigid arms are considered in, for example, [6, 11]; rigid arms carry geometric constraints that may impede two complementary cohesive-ends to bond together.

A complex assembled from branched junction molecules with flexible arms can be modeled by a graph allowing loops, multiple edges and half-edges: a vertex of degree k represents a branched junction molecule with k arms, and two vertices have a number of edges between them that is equal to the number of connections between the corresponding branched junction molecules. Recall that a *half-edge* of a graph consists of exactly one vertex and every edge uv can be thought as the join of the half-edges (u, uv), (v, uv) that are incident to u, v, respectively. In the language of graphs, a branched junction molecule is called a *tile* and is represented by a vertex with labeled half-edges [3, 4, 5, 11, 12]. The labels represent the *cohesive-end* and belong to a set $\{a, \hat{a} : a \in \Sigma\}$, where Σ is a finite set of symbols, and complementary cohesive-end are denoted by hatted and unhatted copies of the same letter, so that $\hat{\hat{a}} = a$ for every $a \in \Sigma$, with $a \neq \hat{a}$. Because the arms of the molecules are assumed to be flexible, a tile can be specified by the multiset consisting of the labels on its half-edges. Two tiles are of the same *tile type* if they are represented by the same multiset. We can create an edge between two tiles t and t' if and only if t has a half-edge labeled by, say a, and t' has a half-edge labeled by $\hat{a}$; the edge thus obtained is said to be a *bond-edge of type a* (such an edge represents an attachment of the molecules the tiles represent through arms with complementary cohesive-ends). Figure 1 describes in short the join of branched junction molecules with flexible arms and the corresponding representation by graphs. A structure assembled from branched junction molecules is a *complete complex* if it has no branched junction molecule with unmatched cohesive-ends; thus in the corresponding graph, called a *complete complex* by analogy, unmatched half-edges are not allowed.

For a vertex v of a graph G – allowing loops, multiple edges and half-edges – the set (or multiset) of its incident half-edges includes the half-edges (v, uv), where uv is an edge of G joining the vertices u, v. A set of tile types, called a *pot*, *realizes* a graph G if we can assign a tile type in the pot to each vertex v of G and its incident half-edges in such a way that: (i) there is a bijection between half-edges of v and labels of the corresponding tile type; (ii) each edge receives both an unhatted and hatted copy of the same letter on its half-edges [5, 3]. A target graph G is efficiently constructed if the number of tile types or bond-edge types, in a pot realizing G, are minimized. The problem of efficiently realizing a graph G leads to the definition of



(a) (b) (c)

Figure 1: (a) A schematic representation of two branched junction molecules, with three flexible arms, that are joined together by arms with complementary cohesive-ends. (b) The two molecules can be represented as vertices with labeled half-edges, where half-edges correspond to the arms of the molecules, labels correspond to the cohesive-ends (for instance, label a and $\hat{a}$ correspond to the cohesive-ends "CCA" and "GGT", respectively). (c) We can join the two half-edges with labels a, $\hat{a}$ and form a bond-edge of type a.

two new graph invariants, namely $T(G)$ and $B(G)$, that correspond to the minimum number of tile types and bond-edge types, respectively, required to realize G. Because in an experiment there is an arbitrarily large number of each branched junction molecule, a pot that realizes a graph G may realize other graphs as well, and graphs with fewer vertices are more likely to form [12]. Hence, the problem of determining a pot with the minimum number of tile types or bond-edge types needed to realize a graph G, is considered under three different laboratory settings [3, 4]:

- Scenario 1. The pot realizing G is allowed to realize graphs of order smaller than $|V(G)|$.
- Scenario 2. The pot realizes the graph G and no graph of order smaller than $|V(G)|$.
- Scenario 3. The pot realizes the graph G and no graph of order smaller than $|V(G)|$ or having the same order as G but not isomorphic to G.

The problem is considered for graphs corresponding to complete complexes, because from a pot realizing G it is always possible to obtain graphs with unmatched half-edges and order smaller than $|V(G)|$ (any tile corresponds to an incomplete complex). Ellis-Monaghan et al. [3] provide specific minimum values for $T(G)$ and $B(G)$ for common families of graphs, such as trees, cycles, complete, bipartite and regular graphs, in these three scenarios. Here, we address the problem using edge-colorings of graphs. In Section 2, we show that the problem can be related to some chromatic parameters that are known in literature, such as the *generalized chromatic index* [7] and the *palette index* of a graph [9]. We show that these chromatic parameters can be used to find upper and lower bounds for $T(G)$ in the three scenarios (see Propositions 4 and 5). In Section 4, we give an upper bound for the parameter $B(G)$ in Scenario 2 and 3; $B(G)$ in Scenario 1 is determined in Proposition 2. From the literature, no general strategy for computing $T(G)$ and $B(G)$, where G is an arbitrary graph is known. Our approach holds for arbitrary graphs and yields bounds for $T(G)$ and $B(G)$, which in turn lead to alternative proofs of the findings in [3]. Moreover, we emphasize that the techniques and the results presented here may improve the yields of self-assembly experiments: by our approach we can efficiently construct the target graph and avoid the assembly of undesired structures.

2 From edge-colorings to multi-palettes and tiles.

In this section we present the main definitions to describe the mathematical model for representing the self-assembly by branched junction molecules [3, 4, 5, 12]. Here, however, we introduce these notions in the setting of edge-colorings. This enables us to establish a relation between the minimum number of bond-edge types required to realize a graph G and the generalized chromatic index of G [7]. We also show that the minimum number of tile types needed to realize G is related to the palette index of a simple graph [9].

In our notation, a graph G is connected and allows loops and multiple edges. As remarked in Section 1, an edge $uv \in E(G)$ can be represented as the join of the half-edges (u, uv) and (v, uv) that are incident to u and v, respectively. Throughout the paper, we will refer to the set of half-edges constituting the edges of G as "the half-edges of G". We denote by P_n the path with n edges and $n+1$ vertices; by C_n the cycle of length n. We refer to [1] for graph theory notation and terminology which are not explicitly described in this paper.

Recall that an *edge-coloring* $f : E(G) \to \mathcal{C}$ of a graph G is an assignment of colors to the edges of G. The edge-coloring is said to be *proper* if adjacent edges receive distinct colors. If f uses k distinct colors, then we say that f is a k-edge-coloring. For every color c in the color-set $\mathcal{C}$ of f and for every vertex $v \in V(G)$, we denote by $f_v^{-1}(c)$ the number of edges of G that are incident to v and are colored with c by f. By this definition, we can say that an edge-coloring f defines at each vertex $v \in V(G)$ a positive integer $m_f(v)$ given by $m_f(v) = \max_{c \in \mathcal{C}}\{f_v^{-1}(c)\}$. Notice that $m_f(v) \leq d(v)$, where $d(v)$ is the degree of v in G. Moreover, f is proper if and only if $m_f(v) = 1$ for every $v \in V(G)$.

Let $m : V(G) \to \mathbb{Z}^+$ be a function such that $m(v) \leq d(v)$ for every $v \in V(G)$. We say that f is an *edge-coloring of type* m if $m_f(v) \leq m(v)$ for every $v \in V(G)$. We denote by $\chi'_m(G)$ the smallest positive integer k

for which a k-edge-coloring of type m exists for G. Notice that in [7] an edge-coloring of type m is called a proper edge-coloring. To avoid misunderstanding with the classical definition of proper edge-coloring, we prefer to adopt the terminology of edge-coloring of type m when $m(v) \neq 1$ for at least one vertex v. Moreover, in [7] the parameter $\chi'_m(G)$ is defined for graphs that allows multiple edges but no loops (loops are allowed in our definition). As in [7], the parameter $\chi'_m(G)$ will be called the *generalized chromatic index of* G.

An edge-coloring f of type m defines at each vertex $v \in V(G)$ the multiset $P_f(v)$ of colors of edges incident to v. Throughout the paper, a multiple entry in a multiset will be denoted by the exponent to the corresponding element; so if $h \geq 1$ edges incident to v are colored by a, then we set $a^h \in P_f(v)$. Notice that $h \leq m(v)$. The multiset $P_f(v)$ will be called the *multi-palette of* v with respect to f. We denote by $\mathcal{P}_f$ the set of distinct multi-palettes of f and say that f has $|\mathcal{P}_f|$ multi-palettes. We define the *multi-palette index of* G, denoted by $\check{s}_m(G)$, as the minimum number of multi-palettes taken over the set of all possible edge-colorings of G of type m, that is,

$$\check{s}_m(G) = \min\{|\mathcal{P}_f| : f \text{ edge-coloring of } G \text{ of type } m\}.$$

We give an example for illustrating the definition of edge-coloring of type m, $\chi'_m(G)$ and $\check{s}_m(G)$.

Example 1. In Figure 2(a) it is depicted a graph G having an edge-coloring of type m, where $m(v_i) = 2$ for every $1 \leq i \leq 5$. The set $\mathcal{P}_f$ of distinct multi-palettes of f consists of the following elements: $\mathcal{P}_f = \{\{a^2, b^2\},\{a^2\}, \{a^2, b\}\}$, where $P_f(v_1) = \{a^2, b^2\}$, $P_f(v_2) = P_f(v_5) = \{a^2\}$, $P_f(v_3) = P_f(v_4) = \{a^2, b\}$. Since the degree-set of the graph has size 3, the multi-palette index $\check{s}_m(G)$ is at least 3; by the cardinality of $\mathcal{P}_f$, the multi-palette index $\check{s}_m(G)$ is exactly 3. As for the generalized chromatic index $\chi'_m(G)$, we have $\chi'_m(G) \geq 2$, since v_1 has degree 4 and $m(v_1) = 2$; by the edge-coloring f in Figure 2(a) that uses exactly two colors, the generalized chromatic index $\chi'_m(G)$ is exactly 2.

The notions of multi-palette and multi-palette index appear here for the first time and are a generalization of the notions of palette and palette index of a simple graph that were introduced in [9]. In fact, given a simple graph G we can consider its edge-colorings of type m with $m(v) = 1$ for every $v \in V(G)$. Then each multi-palette is a set and $\check{s}_m(G) = \check{s}(G)$, where $\check{s}(G)$ is the palette index of G.

If uv is an edge of G with $f(uv) = a$, then its half-edges (u, uv) and (v, uv) can be labeled by a and $\hat{a}$, respectively, or vice versa. As a consequence, an edge-coloring f defines at each vertex $v \in V(G)$ the multiset $t_f(v)$ of labels of the half-edges incident to v, as follows: if uv is an edge of G with $f(uv) = a$, then $x \in t_f(v)$ if and only if $y \in t_f(u)$, where $\{x, y\} = \{a, \hat{a}\}$. We

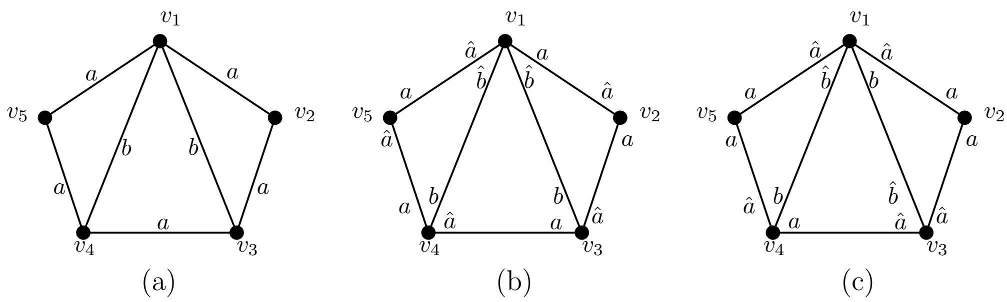


Figure 2: (a) A graph having an edge-coloring f of type m, where $m(v_i) = 2$ for every $1 \leq i \leq 5$; the vertices have the following multi-palettes with respect to f: $P_f(v_1) = \{a^2, b^2\}$, $P_f(v_2) = P_f(v_5) = \{a^2\}$, $P_f(v_3) = P_f(v_4) = \{a^2, b\}$. (b)-(c) Two distinct labelings of the half-edges of the graph providing two distinct pots associated to f: $\{\{a, \hat{a}, \hat{b}^2\}, \{a, \hat{a}\}, \{a, \hat{a}, b\}\}$ pot in case (b); $\{\{\hat{a}^2, b, \hat{b}\}, \{a^2\}, \{\hat{a}^2, \hat{b}\}, \{a, \hat{a}, b\}\}$ pot in case (c) (see Example 1).

call $t_f(v)$ the *tile type of v with respect to f*. Every labeling of the half-edges of G defines a set $\mathcal{T}_f$ of distinct tile types which is associated to f; the set $\mathcal{T}_f$ will be called a *pot associated to f* and accordingly a vertex with labeled half-edges will be called a *tile with respect to f*. Note that there might be different pots associated to the same edge-coloring f, since we can label the half-edges incident to a vertex v in different ways. A pot $\mathcal{T}_f$ associated to an edge-coloring f is characterized by the property that for each label, say a, that appears in any tile type $t \in \mathcal{T}_f$ there exists a label $\hat{a}$ (the complement of a) that appears in some tile type $t' \in \mathcal{T}_f$ (possibly $t = t'$), and vice versa.

Example 2. According to the edge-coloring f in Figure 2(a), we label the two half-edges forming the edge v_1v_5 colored by a with the labels a and $\hat{a}$. Consequently, exactly one of the vertices incident to v_1v_5 has tile type with respect to f containing the label a; the other vertex has tile type containing the label $\hat{a}$. Analogously, for the half-edges forming the remaining edges colored with a and b by f.

The labeling in Figure 2(b) yields the following tile types with respect to f: $t_f(v_1) = \{a, \hat{a}, \hat{b}^2\}$, $t_f(v_2) = t_f(v_5) = \{\hat{a}^2\}$, $t_f(v_3) = t_f(v_4) = \{a, \hat{a}, b\}$; whence the pot $\{\{a, \hat{a}, \hat{b}^2\}, \{a, \hat{a}\}, \{a, \hat{a}, b\}\}\}$ which is associated to f.

The labeling in Figure 2(c) yields the following tile types with respect to f: $t_f(v_1) = \{\hat{a}^2, b, \hat{b}\}$, $t_f(v_2) = t_f(v_5) = \{a^2\}$, $t_f(v_3) = \{\hat{a}^2, \hat{b}\}$, $t_f(v_5) = \{a, \hat{a}, b\}$; whence the pot $\{\{\hat{a}^2, b, \hat{b}\}, \{a^2\}, \{\hat{a}^2, \hat{b}\}, \{a, \hat{a}, b\}\}$ which is associated to f.

Any finite multiset of hatted and unhatted labels can be thought as a tile type with respect to a suitable edge-coloring of a graph, for instance of the star with as many edges as the number of labels in the multiset; the unhatted version of each label corresponds to a color. We will use the term *tile type* to refer to a finite multiset of hatted and unhatted labels (that we interpret as hatted and unhatted colors) and a vertex with labeled half-edges will be simply called a *tile*. The definition of a "tile type" (respectively, "tile") generalizes that one of a "tile type of v with respect to f" (respectively, "tile with respect to f"). We can thus generalize the notion of a "pot associated to f" to that one of a *pot*, that is, any finite set $\mathcal{T}$ of tile types. By the definition of "tile type", each element of a pot can be viewed as a tile type with respect to a suitable edge-coloring of a star having a suitable number of edges. It might happen that no subset of the pot corresponds to a pot associated to an edge-coloring f of a star or of any graph. We say that a pot $\mathcal{T}$ *realizes* the graph G or, equivalently, that G can be constructed from $\mathcal{T}$, if $\mathcal{T}$ contains a pot associated to a suitable edge-coloring of G. The definition of $\mathcal{T}$ realizing a graph G means that there exists a set of tiles, whose tile type is in $\mathcal{T}$, for which it is possible to match the half-edges with complementary labels in such a way that the resulting graph is non-empty, has no unmatched half-edges and is isomorphic to G. As remarked in Section 1, a non-empty graph with no unmatched half-edges is called a *complete complex*. Observe that, in a complete complex G, the number of half-edges of G that are labeled by, say a, is equal to the number of half-edges that are labeled by $\hat{a}$.

Notice that the definitions of tile, tile type and pot introduced above agree with the ones presented in [3, 4, 5, 12], but are obtained by a new approach employing edge-colorings.

3 Preliminary results

Given a pot $\mathcal{T}_f$ associated to an edge-coloring f of G, the cardinality of $\mathcal{T}_f$ represents the number of tile types that are used in the construction of G; on the other hand, the colors of f or, equivalently, the labels appearing in the elements of $\mathcal{T}_f$ (without distinction between hatted or not) correspond to the *bond-edge types* used to realize G. For $i = 1, 2, 3$, let $B_i(G)$ and $T_i(G)$ denote the minimum number of bond-edge types and tile types, respectively, required to realize the graph G according to Scenario i. It is easy to see that $B_1(G) \leq B_2(G) \leq B_3(G)$ and $T_1(G) \leq T_2(G) \leq T_3(G)$ [3]. In this section, we provide some preliminary results for these parameters.

Proposition 1. *A graph G can be constructed from k bond-edge types if and only if there exists a k-edge-coloring of type m, where m is a suitable function from $V(G)$ to $\mathbb{Z}^+$ such that $m(v) \leq d(v)$ for every $v \in V(G)$.* $\square$

As a direct consequence of Proposition 1, we have the following results for $B_1(G)$ and $B_2(G)$.

Proposition 2. *Let G be a graph. For $i = 1, 2, 3$, we have $B_i(G) \geq \chi'_m(G)$, where m is a suitable function from $V(G)$ to $\mathbb{Z}^+$ such that $m(v) \leq d(v)$ for every $v \in V(G)$. In particular, $B_1(G) = \chi'_m(G) = 1$, where $m(v) = d(v)$ for every $v \in V(G)$.*

Proof. By definition of $B_i(G)$, the graph G can be constructed from $B_i(G)$ bond-edge types, $i = 1, 2, 3$. By Proposition 1, there exists a $B_i(G)$-edge-coloring of type m, where m is a suitable function from $V(G)$ to $\mathbb{Z}^+$ such that $m(v) \leq d(v)$ for every $v \in V(G)$. By definition of $\chi'_m(G)$, we have $B_i(G) \geq \chi'_m(G)$. The edge-set of an arbitrary graph G can be colored by just one color, that is, G has a 1-edge-coloring of type m, where $m(v) = d(v)$ for every $v \in V(G)$. Whence $\chi'_m(G) = 1$ where $m(v) = d(v)$ for every $v \in V(G)$. By Proposition 1, the graph G can be constructed from exactly one bond-edge type. This is equivalent to say that $B_1(G) = \chi'_m(G) = 1$, where $m(v) = d(v)$ for every $v \in V(G)$. □

The result $B_1(G) = 1$ for every graph G has been also obtained in [3].

We recall that a *spanning subgraph* of a graph G is a subgraph of G having the same vertex-set as G. The following result will be used in Section 4.

Proposition 3. *Let G be a graph and let G^* be a spanning subgraph of G. Then $B_2(G) \leq B_2(G^*) + 1$.*

Proof. Set $B_2(G^*) = k$. By Proposition 1, there exists a k-edge-coloring f_1 of G^*. We denote by $\{a_1, \ldots, a_k\}$ the color-set of f_1. By definition of $B_2(G^*)$, the edge-coloring f_1 provides a pot $\mathcal{T}_{f_1}$ that realizes no graph of order smaller than $|V(G)|$. We define a $(k+1)$-edge-coloring f of G as follows: if $uv \in E(G^*)$, then we set $f(uv) = f_1(uv)$; if $uv \notin E(G^*)$, then we set $f(uv) = a_{k+1}$, where a_{k+1} is a color not belonging to $\{a_1, \ldots, a_k\}$. For every $v \in V(G)$ we set $t_f(v) = t_{f_1}(v) \cup \{a^i_{k+1}, \hat{a}^j_{k+1}\}$, where i, j are non-negative integers such that $i + j$ corresponds to the number of edges in $E(G) \smallsetminus E(G^*)$ that are incident to v. A pot $\mathcal{T}_f$ is thus defined. Since each tile type of $\mathcal{T}_f$ contains a tile type of $\mathcal{T}_{f_1}$ and $\mathcal{T}_{f_1}$ realizes no graph of order smaller than $|V(G)|$, then so does the pot $\mathcal{T}_f$. It is thus proved that $B_2(G) \leq B_2(G^*) + 1$. □

Proposition 4. *Let G be a graph and let f be an edge-coloring of G. For every pot $\mathcal{T}_f$ associated to f, we have*

$$|\mathcal{P}_f| \leq |\mathcal{T}_f| \leq \sum_{P \in \mathcal{P}_f} 2^{|P|}.$$

Proof. By definition of tile type, every multi-palette of f gives rise to a tile type. Since two elements of $\mathcal{P}_f$ differ on at least one color, they give rise to distinct tile types. Therefore, $|\mathcal{P}_f| \leq |\mathcal{T}_f|$. Every multi-palette $P \in \mathcal{P}_f$ can be split into at most $2^{|P|}$ tile types, since every color $a \in P$ can be split into the 2 labels a and $\hat{a}$. □

Remark 1. If at least one multi-palette P contains repeated colors, then the cardinality of $\mathcal{T}_f$ is smaller than $\sum_{P \in \mathcal{P}_f} 2^{|P|}$. As an example, if $P = \{a^3\}$, then P cannot be split into 2^3 tile types, but it provides at most 4 distinct tile types. Nevertheless, if no multi-palette of f contains repeated colors, then the upper bound in Proposition 4 is tight. As an example, assume that G is a cycle with an even number of vertices. We color alternately its edges by the colors a and b. We obtain a proper edge-coloring f such that $\mathcal{P}_f$ consists of the palette $P = \{a, b\}$. It is easy to verify that we can label the half-edges of G so that the palette P can be split into exactly 2^2 tile types, thus obtaining a pot $\mathcal{T}_f$ whose cardinality is $\sum_{P \in \mathcal{P}_f} 2^{|P|} = 2^2$.

Proposition 5. *Let G be a graph. For $i = 1, 2, 3$, we have $T_i(G) = |\mathcal{T}_f| \geq \check{s}_m(G)$, where f is an edge-coloring of G of type m and m is a suitable function $m : V(G) \to \mathbb{Z}^+$ such that $m(v) \leq d(v)$ for every $v \in V(G)$.*

Proof. By definition of $T_i(G)$ and by Proposition 1, there exists an edge-coloring f of G of type m, where m is a suitable function $m : V(G) \to \mathbb{Z}^+$ with $m(v) \leq d(v)$ for every $v \in V(G)$, such that $T_i(G) = |\mathcal{T}_f|$. By Proposition 4 and by the definition of $\check{s}_m(G)$, we have $T_i(G) = |\mathcal{T}_f| \geq |\mathcal{P}_f| \geq \check{s}_m(G)$. $\square$

Lemma 1. *Let G be a graph and let f be a $B_3(G)$-edge-coloring of G providing a pot $\mathcal{T}_f$ realizing the graph G in Scenario 3. The following properties hold:*

(i) *if G has no loops and there exists $v \in V(G)$ such that $a^h \in P_f(v)$, with $h > 1$, then $t_f(v)$ does not contain both labels a, $\hat{a}$;*

(ii) *if G is simple and there exist $u, v \in V(G)$ such that $a^h \in t_f(u)$, $\hat{a}^s \in t_f(v)$, with $h, s \geq 1$, then at least one of the integers h, s is 1;*

(iii) *if G is simple and there exist $uu_1, uu_2, vv_1, vv_2 \in E(G)$ that are colored by the same color, then for $i = 1, 2$ the edges uv_i, $vu_i \notin E(G)$;*

(iv) *if G has no loops and $uv \in E(G)$, then $t_f(u) \neq t_f(v)$.*

Proof. We prove property (i). Suppose that $t_f(v)$ contains both labels a and $\hat{a}$. Let vv_1, $vv_2 \in E(G)$ such that the half-edges (v, vv_1), (v, vv_2) are labeled by a, $\hat{a}$, respectively (v_1, v_2 are not necessarily distinct). The half-edges (v_1, vv_1), (v_2, vv_2) are labeled by $\hat{a}$, a, respectively. The pot $\mathcal{T}_f$ realizes the graph K that can be obtained from G by removing the edges vv_1, vv_2 and by adding the edges v_1v_2, vv, where vv is a loop incident to v (if $v_1 = v_2$, then v_1v_2 is a loop). The graph K is not isomorphic to G, since G has no loops. Moreover, $|V(K)| = |V(G)|$. That yields a contradiction, since $\mathcal{T}_f$ realizes the graph G and satisfies the conditions in Scenario 3. Hence property (i) holds.

The proof of properties (ii), (iii) and (iv) is similar to the proof of property (i) and will be omitted. $\square$

It is straightforward to see that the next statement is a consequence of property (iv) of Lemma 1.

Corollary 1. $T_3(K_n) = n$. $\square$

4 Bounds for $B_2(G)$ and $B_3(G)$ from graph decompositions.

We say that a graph G has a *decomposition* $\mathcal{D}$, if $\mathcal{D}$ is a collection of subgraphs of G that partition the edge-set of G. Two graphs G_1, G_2 have the same decomposition $\mathcal{D}$, if there exists a decomposition $\mathcal{D}_i$ of G_i, $i = 1, 2$, and a one-to-one correspondence $\phi : \mathcal{D} \to \mathcal{D}_i$ that maps each subgraph $H \in \mathcal{D}$ to a subgraph $\phi(H) \in \mathcal{D}_i$ such that H and $\phi(H)$ are isomorphic. Graphs having the same decomposition are not necessarily isomorphic, see for instance the graphs in Figure 3.

A decomposition $\mathcal{D}$ of a graph G defines a pot $\mathcal{T}_{f_\mathcal{D}}$ which is associated to an edge-coloring $f_\mathcal{D}$ of G and realizes the graph G, as we are going to explain. We color the elements of $\mathcal{D}$ by disjoint color-sets. For every $H \in \mathcal{D}$, we consider an edge-coloring f_H of H with color-set $\mathcal{C}_H$ and associated pot $\mathcal{T}_{f_H}$. The edge-coloring $f_\mathcal{D} : E(G) \to \cup_{H \in \mathcal{D}} \mathcal{C}_H$, defined by $f_\mathcal{D}(e) = f_H(e)$ if $e \in E(H)$, is an edge-coloring of G providing the pot $\mathcal{T}_{f_\mathcal{D}} = \{t_1, \ldots, t_{\tau(\mathcal{D})}\}$, where $t_i = t_f(v_i) = \cup_{\substack{H \in \mathcal{D} \\ v_i \in V(H)}} t_{f_H}(v_i)$ for some vertex $v_i \in V(G)$, $1 \leq i \leq \tau(\mathcal{D})$. We say that the edge-coloring $f_\mathcal{D}$ and the associated pot $\mathcal{T}_{f_\mathcal{D}}$ are *obtained by combining the edge-colorings* f_H and *the associated pots* $\mathcal{T}_{f_H}$, where $H \in \mathcal{D}$. A pot $\mathcal{T}_{f_\mathcal{D}}$ arising from a decomposition $\mathcal{D}$ might realize non-isomorphic graphs, see for instance the graphs in Figures 3 and 4 that are considered in Examples 3 and 4, respectively.

The next proposition provides a method for constructing a pot realizing a graph G and no graph of order smaller than $|V(G)|$, starting from a decomposition $\mathcal{D}$ of G; hence it can be used to find an upper bound for $B_2(G)$. For instance, for Hamiltonian graphs of order n it provides the upper bound $B_2(G) \leq \lceil n/2 \rceil + 1$ (see Corollary 4). Corollaries 2, 3, 5 and 6 show that Proposition 6 has stronger implications, since it also gives the exact value of $B_2(G)$ and $B_3(G)$ for some notable classes of graphs– cycles, complete graphs and complete bipartite graphs.

The statement of Proposition 6 is as general as possible, that is, it employs a decomposition $\mathcal{D}$ into arbitrary subgraphs H, so that it can be applied to any graph G; the subset $\mathcal{D}^* \subseteq \mathcal{D}$ plays the role of a subset of subgraphs H whose union spans the graph G; the subset $\mathcal{T}^*$ is a selection of tile types in each $H \in \mathcal{D}^*$ that uniquely defines a partition of the tile types of the whole graph G. The upper bound obtainable from Proposition 6 depends from the choice of the subgraphs H and in view of reaching the exact value of $B_2(G)$, it suggests to select the subgraphs H that make the value of $\sum_{H\in\mathcal{D}} |\mathcal{C}_h|$ as small as possible.

Some further notations are in order. If G can be constructed from a pot $\mathcal{T}$ containing a pot associated to an edge-coloring f of G and for $t \in \mathcal{T}$ there are exactly $n_t \geq 0$ vertices of $V(G)$ having tile type t, then we denote the corresponding multiset of tile types by $\mathcal{M}_f(G) = \{t^{n_t} : t \in \mathcal{T}, n_t \geq 0\}$. Notice that $\sum_{t\in\mathcal{T}} n_t = |V(G)|$.

Let G and L be graphs that can be constructed from the same pot $\mathcal{T}$ containing a pot associated to an edge-coloring of G (respectively, of L); for simplicity, we denote both edge-colorings by f and set $\mathcal{M}_f(G) = \{t^{n_t} : t \in \mathcal{T}, n_t \geq 0\}$, $\mathcal{M}_f(L) = \{t^{m_t} : t \in \mathcal{T}, m_t \geq 0\}$. We say that $\mathcal{M}_f(L)$ contains $\lambda \geq 1$ copies of $\mathcal{M}_f(G)$ if $m_t \geq \lambda \cdot n_t$ for every $t \in \mathcal{T}$.

Proposition 6. *Let G be a connected graph having a decomposition $\mathcal{D}$. For every $H \in \mathcal{D}$, let f_H be an edge-coloring of H with color-set $\mathcal{C}_H$ and associated pot $\mathcal{T}_{f_H}$. Let $f_\mathcal{D}$ be the edge-coloring of G obtained by combining the edge-colorings f_H and let $\mathcal{T}_{f_\mathcal{D}} = \{t_i : 1 \leq i \leq \tau(\mathcal{D})\}$ be the associated pot obtained by combining the pots $\mathcal{T}_{f_H}$.*

Let $\mathcal{D}^* \subseteq \mathcal{D}$ and $\mathcal{T}^* \subseteq (\cup_{H\in\mathcal{D}^*}\mathcal{T}_{f_H})$ such that $\mathcal{T}^* \cap \mathcal{T}_{f_H} \neq \emptyset$ for every $H \in \mathcal{D}^*$. Assume that $\mathcal{D}^*$ and $\mathcal{T}^*$ define a partition of $\mathcal{T}_{f_\mathcal{D}}$ into the subsets A_t, where $t \in \mathcal{T}^*$ and each A_t consists of the tile types $t_i \in \mathcal{T}_{f_\mathcal{D}}$ containing the tile type $t \in \mathcal{T}^*$. Moreover, the following conditions hold:

(0) *no element of $\mathcal{T}_{f_\mathcal{D}}$ can belong to more than one subset A_t, that is, if $t_i \in A_{t'}$, then t_i contains no tile type $t \in \mathcal{T}^*$, $t \neq t'$;*

(1) *for every $H \in \mathcal{D}^*$, if L_H is a graph that can be constructed from $\mathcal{T}_{f_H}$, then $\mathcal{M}_{f_H}(L_H)$ contains $\lambda_H \geq 1$ copies of $\mathcal{M}_{f_H}(H)$.*

Then $\mathcal{T}_{f_\mathcal{D}}$ realizes no graph of order smaller than $|V(G)|$. Whence $B_2(G) \leq \sum_{H\in\mathcal{D}} |\mathcal{C}_H|$.

Proof. Let L be a graph that can be constructed from $\mathcal{T}_{f_\mathcal{D}}$. We prove that $|V(L)| \geq |V(G)|$. We set $\mathcal{M}_{f_\mathcal{D}}(G) = \{t_i^{n_i} : n_i \geq 0, 1 \leq i \leq \tau(\mathcal{D})\}$, $\mathcal{M}_{f_\mathcal{D}}(L) = \{t_i^{m_i} : m_i \geq 0, 1 \leq i \leq \tau(\mathcal{D})\}$ and denote by L_H the subgraph of L induced by the color-set $\mathcal{C}_H$. By the definition of $\mathcal{T}_{f_\mathcal{D}}$, we can set $n_i > 0$ for every $t_i \in \mathcal{T}_{f_\mathcal{D}}$. Notice that L is the edge-disjoint union of the subgraphs L_H. Firstly, we show that L_H is non-empty, for every $H \in \mathcal{D}$. Suppose, on the contrary, that L_H is non-empty for every $H \in \mathcal{D}'$, where $\mathcal{D}' \subset \mathcal{D}$, whereas L_H is empty for every $H \in \mathcal{D} \smallsetminus \mathcal{D}'$. Hence L is the edge-disjoint union of the graphs L_H with $H \in \mathcal{D}'$ and the tile types of its vertices are obtained from the tile types of the vertices in $\cup_{H\in\mathcal{D}'}V(H)$. Since L is a complete complex, the tile types of its vertices contain no label coming from the color-sets $\mathcal{C}_H$

with $H \in \mathcal{D} \smallsetminus \mathcal{D}'$. Therefore, the set $\cup_{H\in\mathcal{D}'} V(H)$ is a non-empty proper subset of $V(G)$, since G has at least one vertex whose tile type with respect to $f_{\mathcal{D}}$ contains labels from the color-sets $\mathcal{C}_H$ with $H \in \mathcal{D}\smallsetminus\mathcal{D}'$. Consequently, the edge-disjoint union of the graphs $H \in \mathcal{D} \smallsetminus \mathcal{D}'$ is a subgraph of G corresponding to a complete complex. Whence G is disconnected, a contradiction. Hence L_H is non-empty for every $H \in \mathcal{D}$. In particular, L_H is non-empty for every $H \in \mathcal{D}^*$. For $H \in \mathcal{D}^*$, we set $\mathcal{M}_{f_H}(H) = \{t^{n_{H,t}} : t \in \mathcal{T}_{f_H}, n_{H,t} \geq 0\}$, $\mathcal{M}_{f_H}(L_H) = \{t^{m_{H,t}} : t \in \mathcal{T}_{f_H}, m_{H,t} \geq 0\}$.

Since the subsets A_t, $t \in \mathcal{T}^*$, partition $\mathcal{T}_{f_{\mathcal{D}}}$, we can set $|V(G)| = \sum_{i=1}^{\tau(\mathcal{D})} n_i = \sum_{t\in\mathcal{T}^*}\sum_{t_i\in A_t} n_i$ and $|V(L)| = \sum_{i=1}^{\tau(\mathcal{D})} m_i = \sum_{t\in\mathcal{T}^*}\sum_{t_i\in A_t} m_i$. By definition of A_t and property (0), the summations $\sum_{t_i\in A_t} n_i$ and $\sum_{t_i\in A_t} m_i$ correspond to the number of vertices of G and L, respectively, whose tile type $t_{f_{\mathcal{D}}}(v) = t_i$ (for a suitable $t_i \in A_t$, $t \in \mathcal{T}^*$) contains the tile type $t \in \mathcal{T}^*$, where $t \in \mathcal{T}_{f_H}$, for some $H \in \mathcal{D}^*$. The number of vertices of G (respectively, of L) whose tile types $t_{f_{\mathcal{D}}}(v) = t_i$ contains $t \in \mathcal{T}_{f_H}$, $H \in \mathcal{D}^*$, corresponds to the number of vertices of H (respectively, of L_H) having tile type $t_{f_H}(v) = t$, since the multi-palettes of the vertices in $V(G) \smallsetminus V(H)$ (respectively, in $V(L) \smallsetminus V(L_H)$) are disjoint from $\mathcal{C}_H$. Therefore, for every $t \in \mathcal{T}^*$, with $t \in \mathcal{T}_{f_H}$, $H \in \mathcal{D}^*$, we have $\sum_{t_i\in A_t} n_i = n_{H,t}$ and $\sum_{t_i\in A_t} m_i = m_{H,t}$. Whence $|V(G)| = \sum_{\substack{t\in\mathcal{T}^*\\ H\in\mathcal{D}^*}} n_{H,t}$ and $|V(L)| = \sum_{\substack{t\in\mathcal{T}^*\\ H\in\mathcal{D}^*}} m_{H,t}$. Since every subgraph L_H, $H \in \mathcal{D}^*$, is non-empty and property (1) holds, the following inequality holds: $m_{H,t} \geq \lambda_H \cdot n_{H,t} \geq n_{H,t}$ for every $H \in \mathcal{D}^*$. Consequently, $|V(G)| \leq |V(L)|$. It is thus proved that the pot $\mathcal{T}_{f_{\mathcal{D}}}$ realizes the graph G and no graph of order smaller than $|V(G)|$. Whence $B_2(G) \leq \sum_{H\in\mathcal{D}} |\mathcal{C}_H|$. □

Property (1) of Proposition 6 implies that for every $H \in \mathcal{D}^*$ the pot $\mathcal{T}_{f_H}$ realizes the graph H and no graph of order smaller than $|V(H)|$. For the graphs $H \in \mathcal{D} \smallsetminus \mathcal{D}^*$, the pot $\mathcal{T}_{f_H}$ might realize graphs that are not isomorphic to H and, in particular, graphs of order smaller than $|V(H)|$.

In the following examples, we give an application of Proposition 6. In Example 3, we exhibit a graph having a decomposition $\mathcal{D}$ consisting of certain subgraphs; for every $H \in \mathcal{D}$ we provide a pot $\mathcal{T}_{f_H}$ realizing the graph H and no graph of order smaller than $|V(H)|$. We also show that the pot $\mathcal{T}_{f_{\mathcal{D}}}$ realizes graphs that are not isomorphic to G, but have the same order as G and the same decomposition $\mathcal{D}$. In Example 4, we exhibit a graph having a decomposition $\mathcal{D}$ consisting of cycles C_4, C_6 and paths P_4; for every $H \in \mathcal{D}^*$, where $\mathcal{D}^*$ is a proper subset of $\mathcal{D}$, we provide a pot $\mathcal{T}_{f_H}$ realizing the graph H and no graph of order smaller than $|V(H)|$; for $H \in \mathcal{D} \smallsetminus \mathcal{D}^*$, we provide a pot $\mathcal{T}_{f_H}$ realizing the graph H and graphs having order smaller than $|V(H)|$. We also show that, in this case, the pot $\mathcal{T}_{f_{\mathcal{D}}}$ realizes graphs that are not isomorphic to G and have the same order as G, but not the same decomposition $\mathcal{D}$. This follows from the fact that the pot $\mathcal{T}_{f_H}$, for $H \in \mathcal{D} \smallsetminus \mathcal{D}^*$ realizes graphs whose order is smaller than $|V(H)|$.

Example 3. The graph G in Figure 3(a) has a decomposition $\mathcal{D}$ into the subgraphs H_i, $1 \leq i \leq 5$, defined in Figure 3. We use the decomposition $\mathcal{D}$ to define a pot $\mathcal{T}_{f_\mathcal{D}}$ realizing the graph G and no graph of order smaller than $|V(G)| = 9$. We color the subgraphs H_i by disjoint color-sets. For $i = 1, 2, 3, 5$, we denote by f_{H_i} the edge-coloring of H_i that colors each edge of H_i by color a_i. We denote by f_{H_4} the edge-coloring of H_4 with color-set $\{b_1, b_2, b_3\}$ that colors the edges incident to v_5 by color b_2; the remaining edges incident to v_4, v_6 by color b_1; and the edge v_7v_8 by b_3. We can label the half-edges of each H_i and define the pot $\mathcal{T}_{f_{H_i}}$ associated to the edge-coloring f_i as follows:

- $\mathcal{T}_{f_{H_1}} = \{\{a_1^3\}, \{\hat{a}_1^3\}\}$; $\mathcal{T}_{f_{H_2}} = \{\{a_2^3\}, \{\hat{a}_2\}\}$; $\mathcal{T}_{f_{H_3}} = \{\{a_3^3\}, \{\hat{a}_3^2\}, \{\hat{a}_3\}\}$;
- $T_{f_{H_4}} = \{\{b_1, b_2\}, \{\hat{b}_2^2\}, \{\hat{b}_1, b_3\}, \{\hat{b}_1, \hat{b}_3\}\}$; $\mathcal{T}_{f_{H_5}} = \{\{a_5^2\}, \{\hat{a}_5^2\}\}$.

It is easy to see that each pot $\mathcal{T}_{f_{H_i}}$, $1 \leq i \leq 5$, realizes the graph H_i and no graph of order smaller than $|V(H_i)|$. Combining the pots $\mathcal{T}_{f_{H_i}}$, we obtain the pot $\mathcal{T}_{f_\mathcal{D}} = \{\{\hat{a}_1^3, \hat{a}_2\}$, $\{\hat{a}_2, \hat{a}_3^2\}$, $\{\hat{a}_2, \hat{a}_3\}$, $\{a_1^3, b_1, b_2\}$, $\{a_2^3, \hat{b}_2^2\}$, $\{a_3^3, b_1, b_2\}$, $\{\hat{b}_1, b_3\}$, $\{\hat{b}_1, \hat{b}_3, a_5^2\}$, $\{\hat{a}_5^2\}\}$ (see also Figure 3) that realizes the graph G. We now prove that it realizes no graph of order smaller than $|V(G)| = 9$ by showing that there exists a partition of $\mathcal{T}_{f_\mathcal{D}}$ that satisfies properties (0) and (1) of Proposition 6.

Set $\mathcal{D}^* = \{H_2, H_4, H_5\}$ and $\mathcal{T}^* = \{\{\hat{a}_2\}$, $\{b_1, b_2\}$, $\{\hat{b}_2^2\}$, $\{\hat{b}_1, b_3\}$, $\{\hat{a}_5^2\}$, $\{a_5^2\}\}$. The elements of $\mathcal{T}_{f_\mathcal{D}}$ can be partitioned into the following subsets A_t, $t \in \mathcal{T}^*$:

- $A_{\{\hat{a}_2\}} = \{\{\hat{a}_1^3, \hat{a}_2\}, \{\hat{a}_2, \hat{a}_3^2\}, \{\hat{a}_2, \hat{a}_3\}\}$;
- $A_{\{b_1,b_2\}} = \{\{a_1^3, b_1, b_2\}, \{a_3^3, b_1, b_2\}\}$; $A_{\{\hat{b}_2^2\}} = \{\{a_2^3, \hat{b}_2^2\}\}$;
- $A_{\{\hat{b}_1,b_3\}} = \{\{\hat{b}_1, b_3\}\}$; $A_{\{\hat{a}_5^2\}} = \{\{\hat{a}_5^2\}\}$; $A_{\{a_5^2\}} = \{\{\hat{b}_1, \hat{b}_3, a_5^2\}\}$.

Property (0) of Proposition 6 is easily satisfied: no element of $\mathcal{T}_{f_\mathcal{D}}$ can belong to more than one subset A_t.

An easy counting argument shows that for every $H \in \mathcal{D}^*$, if L_H can be constructed from $\mathcal{T}_{f_H}$, then $\mathcal{M}_{f_H}(L_H)$ contains $\lambda_H \geq 1$ copies of $\mathcal{M}_{f_H}(H)$. For instance, for $H = H_4$ we have $\mathcal{M}_{f_{H_4}}(H_4) = \{\{b_1, b_2\}^2$, $\{\hat{b}_2^2\}^1$, $\{\hat{b}_1, b_3\}^1$, $\{\hat{b}_1, \hat{b}_3\}^1\}$ and we can set $\mathcal{M}_{f_{H_4}}(L_{H_4})$= $\{\{b_1, b_2\}^{m_1}$, $\{\hat{b}_2^2\}^{m_2}$, $\{\hat{b}_1, b_3\}^{m_3}$, $\{\hat{b}_1, \hat{b}_3\}^{m_4} : m_i \geq 0, 1 \leq i \leq 4\}$. Since the number of half-edges in L_{H_4} that are labeled by b_i, $i = 1, 2, 3$, is equal to the number of half-edges in L_{H_4} that are labeled by $\hat{b}_i$, the following equalities hold: $m_1 = m_3 + m_4$; $m_1 = 2m_2$; $m_3 = m_4$. Whence $m_1 = 2m_4$ and $m_2 = m_3 = m_4$, that is, $\mathcal{M}_{f_{H_4}}(L_{H_4})$ contains $\lambda_H = m_4 \geq 1$ copies of $\mathcal{M}_{f_{H_4}}(H_4)$. Analogously, for the graph L_H that can be constructed from the pot $\mathcal{T}_{f_H}$ with $H \in \mathcal{D}^*$,

$H \neq H_4$. Hence, property (1) of Proposition 6 is satisfied. Since Proposition 6 holds, $B_2(G) \leq 7$.

The pot $\mathcal{T}_{f_\mathcal{D}}$ also realizes graphs that are not isomorphic to the graph in Figure 3(a), for instance the graph in Figure 3(b). Notice that the graphs in Figure 3 have the same decomposition $\mathcal{D} = \{H_i : 1 \leq i \leq 5\}$.

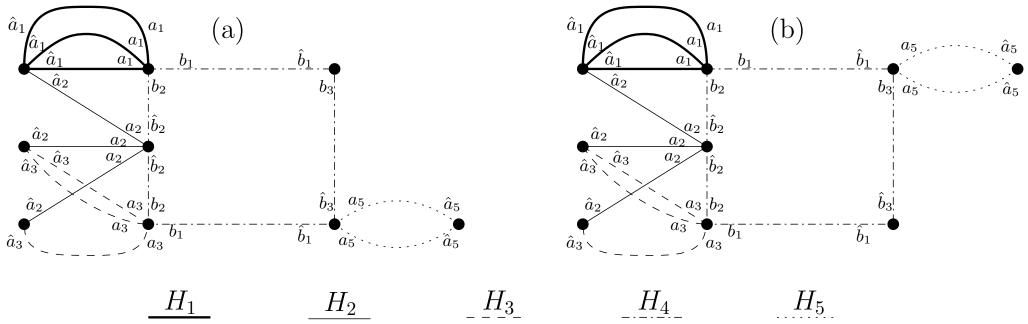


Figure 3: Two non-isomorphic graphs of order 9 having a decomposition $\mathcal{D}$ into the subgraphs H_i, $1 \leq i \leq 5$, that can be constructed from the same pot $\mathcal{T}_{f_\mathcal{D}} = \{\{\hat{a}_1^3, \hat{a}_2\}, \{\hat{a}_2, \hat{a}_3^2\}, \{\hat{a}_2, \hat{a}_3\}, \{a_1^3, b_1, b_2\}, \{a_2^3, \hat{b}_2^2\}, \{a_3^3, b_1, b_2\}, \{\hat{b}_1, b_3\}, \{\hat{b}_1, \hat{b}_3, a_5^2\}, \{\hat{a}_5^2\}\}$ (see Example 3).

Example 4. The graph G in Figure 4(a) has a decomposition $\mathcal{D}$ into the subgraphs H_i, $i = 1, 2, 3$, where H_1 is a cycle C_4; H_2 is a path P_4; and H_3 is a cycle C_6. We use the decomposition $\mathcal{D}$ to define a pot $\mathcal{T}_{f_\mathcal{D}}$ realizing the graph G and no graph of order smaller than $|V(G)| = 9$. We color the subgraphs H_i by disjoint color-sets. We denote by f_{H_1} the edge-coloring of H_1 that colors the edges incident to v_1 by color a_1 and the edges incident to v_2 by color a_2; we denote by f_{H_2} the edge-coloring of H_2 that colors the edges incident to v_8 by color b_2 and the remaining edges of H_2 by color b_1; we denote by f_3 the edge-coloring of H_3 that colors the edges incident to v_3 and v_6 by color c_1 and the remaining edges of H_3 by color c_2. We can label the half-edges of each H_i and define the pot $\mathcal{T}_{f_{H_i}}$ associated to the edge-coloring f_{H_i} as follows:

- $\mathcal{T}_{f_{H_1}} = \{\{a_1^2\}, \{\hat{a}_2^2\}, \{\hat{a}_1, a_2\}\}$; $\mathcal{T}_{f_{H_2}} = \{\{b_1\}, \{\hat{b}_1, b_2\}, \{\hat{b}_2^2\}\}$;
- $\mathcal{T}_{f_{H_3}} = \{\{c_1^2\}, \{\hat{c}_1, c_2\}, \{\hat{c}_1, \hat{c}_2\}\}$.

It is easy to see that the pot $\mathcal{T}_{f_{H_i}}$, with $i = 1, 2$, realizes the graph H_i and no graph of order smaller than $|V(H_i)|$. The pot $\mathcal{T}_{f_{H_3}}$ realizes the graph H_3 and graphs of order smaller than $|V(H_3)|$ (for instance, take a complete graph K_3 whose vertices have tile types $\{c_1^2\}$, $\{\hat{c}_1, c_2\}$, $\{\hat{c}_1, \hat{c}_2\}$). Combining the pots $\mathcal{T}_{f_{H_i}}$, we obtain the pot $\mathcal{T}_{f_\mathcal{D}} = \{\{a_1^2, \hat{c}_1, c_2\}, \{\hat{a}_1, a_2, \hat{c}_1, \hat{c}_2\},$

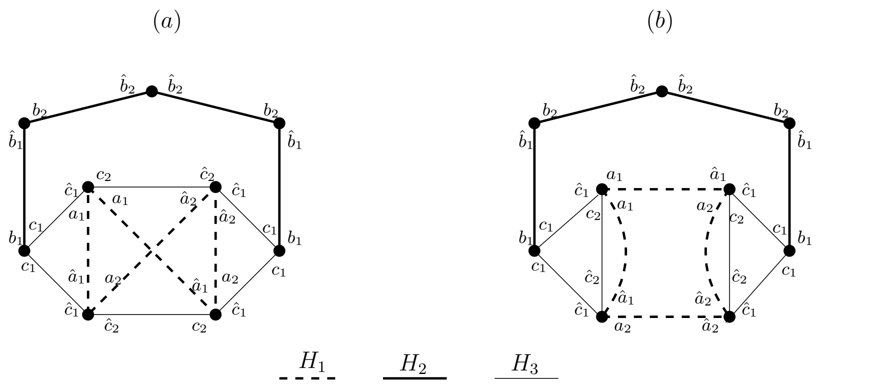
$\{\hat{a}_1, a_2, \hat{c}_1, c_2\}$, $\{\hat{a}_2^2, \hat{c}_1, \hat{c}_2\}$, $\{b_1, c_1^2\}$, $\{\hat{b}_1, b_2\}$, $\{\hat{b}_2^2\}\}$ (see also Figure 4) that realizes the graph G. We now prove that it realizes no graph of order smaller than $|V(G)| = 9$ by showing that there exists a partition of $\mathcal{T}_{f_\mathcal{D}}$ that satisfies properties (0) and (1) of Proposition 6.

Set $\mathcal{D}^* = \{H_1, H_2\}$ and $\mathcal{T}^* = \{\{a_1^2\}, \{\hat{a}_1, a_2\}, \{\hat{a}_2^2\}, \{b_1\}, \{\hat{b}_1, b_2\}, \{\hat{b}_2^2\}\}$. The elements of $\mathcal{T}_{f_\mathcal{D}}$ can be partitioned into the following subsets A_t, $t \in \mathcal{T}^*$:

- $A_{\{a_1^2\}} = \{\{a_1^2, \hat{c}_1, c_2\}\}$; $A_{\{\hat{a}_1, a_2\}} = \{\{\hat{a}_1, a_2, \hat{c}_1, c_2\}, \{\hat{a}_1, a_2, \hat{c}_1, \hat{c}_2\}\}$;
- $A_{\{\hat{a}_2^2\}} = \{\{\hat{a}_2^2, \hat{c}_1, \hat{c}_2\}\}$; $A_{\{b_1\}} = \{\{b_1, c_1^2\}\}$;
- $A_{\{\hat{b}_1, b_2\}} = \{\{\hat{b}_1, b_2\}\}$; $A_{\{\hat{b}_2^2\}} = \{\{\hat{b}_2^2\}\}$.

No element of $\mathcal{T}_{f_\mathcal{D}}$ can belong to more than one subset A_t, hence property (0) of Proposition 6 is satisfied. For every $H \in \mathcal{D}^*$, if L_H can be constructed from $\mathcal{T}_{f_H}$, then $\mathcal{M}_{f_H}(L_H)$ contains $\lambda_H \geq 1$ copies of $\mathcal{M}_{f_H}(H)$; the proof is similar to the proof of Example 3 and will be omitted. Since Proposition 6 is satisfied, $B_2(G) \leq 6$.

The pot $\mathcal{T}_{f_\mathcal{D}}$ also realizes the graph in Figure $4(b)$, which is not isomorphic to the graph in Figure $4(a)$. Notice that the collection $\mathcal{D} = \{H_1, H_2, H_3\} = \{C_4, P_4, C_6\}$ partitions the edge-set of the graph in Figure $4(a)$, but does not partition the edge-set of the graph in Figure $4(b)$.



$\mathcal{T}_{f_\mathcal{D}} = \{\{a_1^2, \hat{c}_1, c_2\}, \{\hat{a}_2^2, \hat{c}_1, \hat{c}_2\}, \{b_1, c_1^2\}, \{\hat{a}_1, a_2, \hat{c}_1, c_2\}, \{\hat{a}_1, a_2, \hat{c}_1, \hat{c}_2\}, \{\hat{b}_1, b_2\}, \{\hat{b}_2^2\}\}$

Figure 4: Two graphs that can be constructed from the same pot $\mathcal{T}_{f_\mathcal{D}}$ arising from the decomposition $\mathcal{D} = \{H_1, H_2, H_3\} = \{C_4, P_4, C_6\}$ of the graph on the left. The collection $\mathcal{D} = \{C_4, P_4, C_6\}$ is not a decomposition for the graph on the right (see Example 4).

In the next results we apply Proposition 6.

Corollary 2.

$$B_2(K_n) = \begin{cases} 1 & \textit{if } n \textit{ is even;} \\ 2 & \textit{if } n \textit{ is odd.} \end{cases} \quad B_2(K_{m,n}) = \begin{cases} 1 & \textit{if } \gcd(m,n) = 1; \\ 2 & \textit{if } \gcd(m,n) > 1. \end{cases}$$

Proof. Set $V(K_n) = \{v_i : 1 \leq i \leq n\}$ and consider the decomposition $\mathcal{D} = \{H_1, H_2\}$, where H_1 is the star $K_{1,n-1}$ with center v_1 and H_2 is the complement of H_1 in K_n, that is, H_2 is the complete graph K_{n-1} on the vertices $V(K_n) \smallsetminus \{v_1\}$. We consider the edge-coloring f_{H_1} of H_1 that colors every edge with a_1 and has $\mathcal{T}_{f_{H_1}} = \{\{a_1^{n-1}\}, \{\hat{a}_1\}\}$ as an associated pot. We color the edges of H_2 with $a_2 \neq a_1$, label the half-edges arbitrarily and consider the resulting pot. Any tile type of a pot $\mathcal{T}_{f_\mathcal{D}}$, obtained from $\mathcal{D}$ by combining $\mathcal{T}_{f_{H_1}}$ together with a pot associated to a coloring of H_2 by color a_2, contains the label a_1^{n-1} or $\hat{a}_1$. Therefore, by setting $\mathcal{D}^* = \{H_1\}$ and $\mathcal{T}^* = \mathcal{T}_{f_{H_1}}$, Proposition 6 is satisfied; whence $B_2(K_n) \leq 2$.

It is easy to see that for even values of n, the pot $\mathcal{T} = \{\{a^{n-1}\}, \{a^{(n/2)-1}, \hat{a}^{n/2}\}\}$ realizes the graph K_n and no graph of order smaller than n; whence $B_2(K_n) = 1$ for even values of n. For odd values of n, $B_2(K_n) = 2$. Suppose, on the contrary, that $B_2(K_n) = 1$ if n is odd, then there exists a 1-edge-coloring f of K_n defining a pot $\mathcal{T}_f$ realizing no graph of order smaller than n. We can set $\mathcal{T}_f = \{\{a^i, \hat{a}^{n-1-i}\} : i \in I\}$, where I is a suitable subset of $\{0, \dots, n-1\}$. For every $i \in I$, we denote by n_i the number of vertices with tile type $\{a^i, \hat{a}^{n-1-i}\}$. Since the total amount of half-edges with label a is equal to the total amount of half-edges with label $\hat{a}$, the relation $\sum_{i \in I}(n - 1 - 2i)n_i = 0$ holds. Whence there exist $h, j \in I$ such that $(n-1-2h) > 0$ and $(n-1-2j) < 0$. We now construct a graph H whose edges are colored by f and whose tile types are contained in $\mathcal{T}_f$. The graph H has $j-(n-1)/2$ vertices whose tile type is $\{a^h, \hat{a}^{n-1-h}\}$ and $(n-1)/2 - h$ vertices whose tile type is $\{a^j, \hat{a}^{n-1-j}\}$. A vertex with tile type $\{a^h, \hat{a}^{n-1-h}\}$ is incident to h loops and to $n-1-2h$ half-edges with label $\hat{a}$. A vertex with tile type $\{a^j, \hat{a}^{n-1-j}\}$ is incident to $n-1-j$ loops and to $2j-n+1$ half-edges with label a. Since $[j-(n-1)/2](n-1-2h) + [(n-1)/2-h](n-1-2j) = 0$, that is, the number of half-edges labeled by a is equal to the number of half-edges that are labeled by $\hat{a}$, we can match them so that the graph H is a complete complex of order $[j-(n-1)/2] + [(n-1)/2-h] = j-h \leq n-1$, since $j \leq n-1$ and $h \geq 0$. That yields a contradiction, since $\mathcal{T}_f$ realizes no graph of order smaller than n. It is thus proved that $B_2(K_n) > 1$ for odd values of n, that is, $B_2(K_n) = 2$.

For the complete graph $K_{m,n}$ with $\gcd(m,n) = 1$, we consider the decomposition $\mathcal{D}$ consisting of the graph $H = K_{m,n}$ itself and the edge-coloring $f_\mathcal{D} = f_H$ that colors every edge of $K_{m,n}$ with color a. We label the half-edges incident to the vertices of degree n by label a; the half-edges incident to the vertices of degree m by label $\hat{a}$. We obtain the pot $\mathcal{T}_{f_\mathcal{D}} = \{\{a^n\}, \{\hat{a}^m\}\}$ which is associated to the coloring $f_\mathcal{D}$. By setting $\mathcal{D}^* = \mathcal{D}$ and $\mathcal{T}^* = \mathcal{T}_{f_\mathcal{D}}$, Proposition 6 is satisfied (condition (1) follows from the assumption $\gcd(m, n) = 1$). Whence $B_2(K_{m,n}) = 1$ if $\gcd(m, n) = 1$.

The complete graph $K_{m,n}$ with $\gcd(m, n) \neq 1$ can be managed analogously to the previous cases. □

Corollary 3. *Let C_n be the cycle on $n \geq 3$ vertices. Then $B_2(C_n) = B_3(C_n) = \lceil n/2 \rceil$.*

Proof. We show that $B_2(C_n) \leq \lceil n/2 \rceil$ by applying Proposition 6. We set $C_n = (v_1, v_2, \ldots, v_n, v_1)$ and find a partition $\mathcal{D}$ of its edge-set into the paths $H_1 = (v_1, v_2, \ldots, v_{n-1})$ and $H_2 = (v_1, v_n, v_{n-1})$. We treat separately the following cases: (1) n even and (2) n odd.

(1) Consider n even. For the path H_1, we take the edge-coloring f_{H_1} with color-set $\mathcal{C}_{H_1} = \{a_i : 1 \leq i \leq (n/2) - 1\}$ and associated pot $\mathcal{T}_{f_{H_1}} = \{\{a_1^2\}, \{\hat{a}_{(n/2)-1}\}, \{\hat{a}_i, a_{i+1}\} : i = 1, \ldots, (n/2) - 2\}$. For the path H_2, we consider the edge-coloring f_{H_2} with color-set $\mathcal{C}_{H_2} = \{a_{n/2}\}$ and associated pot $\mathcal{T}_{f_{H_2}} = \{\{\hat{a}^2_{n/2}\}, \{a_{n/2}\}\}$. Combining the pots $\mathcal{T}_{f_{H_1}}$, $\mathcal{T}_{f_{H_2}}$, we obtain the pot $\mathcal{T}_{f_{\mathcal{D}}} = \{\{a_1^2\}, \{\hat{a}^2_{n/2}\}, \{\hat{a}_i, a_{i+1}\} : i = 1, \ldots, (n/2)-1\}$ realizing the graph C_n.

Set $\mathcal{D}^* = \{H_1, H_2\}$ and $\mathcal{T}^* = \{\{a_1^2\}, \{\hat{a}^2_{n/2}\}, \{a_{n/2}\}, \{\hat{a}_i, a_{i+1}\} : i = 1, \ldots, (n/2) - 2\}$. The elements of $\mathcal{T}_{f_{\mathcal{D}}}$ can be partitioned into the following subsets A_t, $t \in \mathcal{T}^*$: $A_{\{a_1^2\}} = \{\{a_1^2\}\}$; $A_{\{\hat{a}^2_{n/2}\}} = \{\{\hat{a}^2_{n/2}\}\}$; $A_{\{a_{n/2}\}} = \{\{\hat{a}_{(n/2)-1}, a_{n/2}\}\}$; $A_{\{\hat{a}_i, a_{i+1}\}} = \{\{\hat{a}_i, a_{i+1}\}\}$, $1 \leq i \leq (n/2) - 2$. We show that properties (0) and (1) of Proposition 6 are satisfied.

It is easy to see that no element of $\mathcal{T}_{f_{\mathcal{D}}}$ can belong to more than one subset A_t. Hence, property (0) of Proposition 6 is satisfied.

For every $H \in \mathcal{D}^*$, if L_H can be constructed from $\mathcal{T}_{f_H}$, then $\mathcal{M}_{f_H}(L_H)$ contains $\lambda_H \geq 1$ copies of $\mathcal{M}_{f_H}(H)$. For instance, if $H = H_1$, then $\mathcal{M}_{f_H}(H) = \{\{a_1^2\}^1, \{\hat{a}_{(n/2)-1}\}^2, \{\hat{a}_i, a_{i+1}\}^2 : i = 1, \ldots, (n/2) - 2\}$ and we can set $\mathcal{M}_{f_H}(L_H) = \{\{a_1^2\}^\alpha, \{\hat{a}_{(n/2)-1}\}^\beta, \{\hat{a}_i, a_{i+1}\}^{m_i} : \alpha, \beta \geq 0,\ m_i \geq 0, 1 \leq i \leq (n/2)-2\}$. Since the number of half-edges in L_H that are labeled by a_i, $1 \leq i \leq (n/2)-1$, is equal to the number of half-edges in L_H that are labeled by $\hat{a}_i$, the following equalities hold: $2\alpha = m_1$; $\beta = m_{(n/2)-2}$; $m_{i-1} = m_i$ for $2 \leq i \leq (n/2) - 2$. Whence $2\alpha = m_1 = m_2 = \cdots = m_{(n/2)-2} = \beta$, that is, $\mathcal{M}_{f_H}(L_H)$ contains $\alpha \geq 1$ copies of $\mathcal{M}_{f_H}(H)$. Analogously, for $H = H_2$. Hence, property (1) of Proposition 6 is satisfied. Since Proposition 6 holds, $B_2(C_n) \leq |\mathcal{C}_{H_1}| + |\mathcal{C}_{H_2}|$, that is, $B_2(C_n) \leq n/2$ if n is even.

(2) Consider n odd. For the path H_1, we take the edge-coloring f_{H_1} with color-set $\mathcal{C}_{H_1} = \{a_i : 2 \leq i \leq (n+1)/2\}$ and associated pot $\mathcal{T}_{f_{H_1}} = \{\{a_2\}, \{\hat{a}_{(n-1)/2}, \hat{a}_{(n+1)/2}\}, \{\hat{a}_i, a_{i+1}\} : i = 2, \ldots, (n-1)/2\}$. For the path H_2, we consider the edge-coloring f_{H_2} with color-set $\mathcal{C}_{H_2} = \{a_1\}$ and associated pot $\mathcal{T}_{f_{H_2}} = \{\{a_1^2\}, \{\hat{a}_1\}\}$. Combining the pots $\mathcal{T}_{f_{H_1}}$, $\mathcal{T}_{f_{H_2}}$, we obtain the pot

$\mathcal{T}_{f_\mathcal{D}} = \{\{a_1^2\}, \{\hat{a}_{(n-1)/2}, \hat{a}_{(n+1)/2}\}, \{\hat{a}_i, a_{i+1}\} : 1, \leq i \leq (n-1)/2\}$. The rest of the proof is similar to the proof of the case n even. By Proposition 6, $B_2(C_n) \leq (n+1)/2$ if n is odd.

It is thus proved that $B_2(C_n) \leq \lceil n/2 \rceil$. We now show that $B_2(C_n) = \lceil n/2 \rceil$. Suppose that $B_2(C_n) = k < \lceil n/2 \rceil$. By Proposition 1, there exists a k-edge-coloring f of C_n with $k < \lceil n/2 \rceil$. Since $k < \lceil n/2 \rceil$, at least three edges of C_n are colored by the same color a. We can set $f(v_r v_{r+1})= f(v_s v_{s+1})= f(v_t v_{t+1}) = a$, where $1 \leq r < s < t \leq n$. Note that, for $i \in \{r, s, t\}$ the half-edges $(v_i, v_i v_{i+1})$, $(v_{i+1}, v_i v_{i+1})$ are labeled by a, $\hat{a}$ or by $\hat{a}$, a, respectively. Without loss of generality, we can assume that the half-edges $(v_r, v_r v_{r+1})$, $(v_{r+1}, v_r v_{r+1})$ are labeled by a, $\hat{a}$, respectively. If the half-edges $(v_s, v_s v_{s+1})$, $(v_{s+1}, v_s v_{s+1})$ are labeled by a, $\hat{a}$, respectively, then there exists a detachment of the edges of C_n yielding two graphs of order smaller than n, namely, the cycles $C_{s-r} = (v_{r+1}, v_{r+2}, \ldots, v_s, v_{r+1})$ and $C_{n-s+r} = (v_{s+1}, v_{s+2}, \ldots, v_{r-1}, v_r, v_{s+1})$ (C_{s-r} is a loop if $s = r+1$). Analogously, if the half-edges $(v_t, v_t v_{t+1})$, $(v_{t+1}, v_t v_{t+1})$ are labeled by a, $\hat{a}$, respectively. Therefore the half-edges $(v_i, v_i v_{i+1})$, $(v_{i+1}, v_i v_{i+1})$, with $i = s, t$, are labeled by $\hat{a}$, a, respectively. By these assumptions, we find a detachment of the edges of C_n yielding two graphs of order smaller than n, namely, $C_{t-s} = (v_{s+1}, v_{s+2}, \ldots, v_t, v_{s+1})$ and $C_{n-t+s} = (v_{t+1}, v_{t+2}, \ldots, v_{s-1}, v_s, v_{t+1})$ (C_{t-s} is a loop if $t = s+1$). That yields a contradiction, hence $k \geq \lceil n/2 \rceil$. It is thus proved that $\lceil n/2 \rceil \leq B_2(C_n) \leq \lceil n/2 \rceil$, that is, $B_2(C_n) = \lceil n/2 \rceil$.

Finally, we show that $B_3(C_n) = \lceil n/2 \rceil$. As remarked for the case n even, if L is a graph that can be constructed from $\mathcal{T}_{f_\mathcal{D}}$, then $\mathcal{M}_{f_\mathcal{D}}(L) = \{\{a_1^2\}^\alpha, \{\hat{a}_{n/2}^2\}^\beta, \{\hat{a}_i, a_{i+1}\}^{m_i} : \alpha, \beta \geq 0,\ m_i \geq 0, 1 \leq i \leq (n/2)-1\}$ and the equalities $2\alpha = m_1 = m_2 = \cdots = m_{(n/2)-1} = 2\beta$ hold. This is equivalent to say that $\mathcal{M}_{f_\mathcal{D}}(L)$ contains $\alpha \geq 1$ copies of $\mathcal{M}_{f_\mathcal{D}}(C_n) = \{\{a_1^2\}^1, \{\hat{a}_{n/2}^2\}^1, \{\hat{a}_i, a_{i+1}\}^2 : 1 \leq i \leq (n/2)-1\}$. It is easy to see that if $\alpha = 1$, then $\mathcal{M}_{f_\mathcal{D}}(L) = \mathcal{M}_{f_\mathcal{D}}(C_n)$ and L is isomorphic to C_n. Analogously, for the case n odd. The assertion follows. □

Corollary 4. *Let G be a Hamiltonian graph of order n. Then $B_2(G) \leq \lceil n/2 \rceil + 1$.*

Proof. A Hamiltonian cycle of G is a spanning subgraph of G. The assertion follows from Proposition 3 and Corollary 3. □

Corollary 5.

$$B_3(K_n) = n - 1.$$

Proof. We use Proposition 6 to find a pot $\mathcal{T}_{f_\mathcal{D}}$ realizing the graph K_n and no graph of order smaller than n. The graph K_n has a decomposition $\mathcal{D}$ into the subgraphs H_i, $1 \leq i \leq n-1$, where H_i is the star $K_{1,n-i}$. We color the subgraphs H_i by disjoint color-sets $\mathcal{C}_{H_i} = \{a_i\}$ and consider the edge-coloring f_{H_i} that colors each edge of H_i by a_i. The edge-coloring f_{H_i} defines the pot $\mathcal{T}_{f_{H_i}} = \{\{\hat{a}_i^{n-i}\}, \{a_i\}\}$ and $\mathcal{M}_{f_{H_i}}(K_{1,n}) = \{\{\hat{a}_i^{n-i}\}^1, \{a_i\}^{n-i}\}$. Combining the pots $\mathcal{T}_{f_{H_i}}$, we obtain the pot $\mathcal{T}_{f_{\mathcal{D}}} = \{\{\hat{a}_1^{n-1}\}, \{a_1, a_2, \dots, a_{n-1}\}, \{a_1, a_2, \dots, a_{j-1}, \hat{a}_j^{n-j}\} : 2 \le j \le n-1\}$. Notice that $\mathcal{M}_{f_{\mathcal{D}}}(K_n)$ contains exactly one copy of every tile type $t \in \mathcal{T}_{f_{\mathcal{D}}}$, that is, $\mathcal{M}_f(K_n) = \{t^1 : t \in \mathcal{T}_{f_{\mathcal{D}}}\}$.

Set $\mathcal{D}^* = \{H_1\}$ and $\mathcal{T}^* = \{\{a_1\}, \{\hat{a}_1^{n-1}\}\}$. The elements of $\mathcal{T}_{f_{\mathcal{D}}}$ can be partitioned into the following subsets A_t, $t \in \mathcal{T}^*$: $A_{\{a_1\}} = \{\{a_1, a_2, \dots, a_{n-1}\}, \{a_1, a_2, \dots, a_{j-1}, \hat{a}_j^{n-j}\} : 2 \le j \le n-1\}$; $A_{\{\hat{a}_1^{n-1}\}} = \{\{\hat{a}_1^{n-1}\}\}$. No element of $\mathcal{T}_{f_{\mathcal{D}}}$ can belong to more than one subset A_t, that is, property (0) of Proposition 6 is satisfied. Moreover, if L_{H_1} is a graph that can be constructed from $\mathcal{T}_{f_{H_1}}$, then $\mathcal{M}_{f_{H_1}}(L_{H_1})$ contains $\lambda_{H_1} \ge 1$ copies of $\mathcal{M}_{f_{H_1}}(K_{1,n})$. The property follows from the fact that the number of half-edges that are labeled by a_1 is equal to the number of half-edges that are labeled by $\hat{a}_1$, since L_{H_1} is a complete complex. Hence, property (1) of Proposition 6 is satisfied. Since Proposition 6 holds, the pot $\mathcal{T}_{f_{\mathcal{D}}}$ realizes the graph K_n and no graph of order smaller than n.

We now show that if the graph realized by $\mathcal{T}_{f_{\mathcal{D}}}$ has order n, then it is isomorphic to K_n. Let L be a graph that can be constructed from $\mathcal{T}_{f_{\mathcal{D}}}$. We set $\mathcal{M}_{f_{\mathcal{D}}}(L) = \{\{\hat{a}_1^{n-1}\}^{m_1}, \{a_1, a_2, \dots, a_{n-1}\}^{m_n}, \{a_1, a_2, \dots, a_{j-1}, \hat{a}_j^{n-j}\}^{m_j} : 2 \le j \le n-1, m_1, m_n, m_j \ge 0\}$. For every $1 \le i \le n$, the relation $m_i(n-i) = \sum_{j=i+1}^{n} m_j$ holds since the number of half-edges that are labeled by $\hat{a}_i$ is equal to the number of half-edges that are labeled by a_i. Since $|V(L)| = \sum_{j=1}^{i} m_j + \sum_{j=i+1}^{n} m_j$, the above relation can be written as $m_i(n-i) = |V(L)| - \sum_{j=1}^{i} m_j$ or, equivalently, $m_i(n-i+1) = |V(L)| - \sum_{j=1}^{i-1} m_j$. Whence, $m_{i+1}(n-i) = |V(L)| - \sum_{j=1}^{i} m_j = m_i(n-i)$. Therefore, $m_{i+1} = m_i$ for every $1 \le i \le n$ (subscripts are read modulo n). It follows that $|V(L)| = n$ if and only if $\mathcal{M}_{f_{\mathcal{D}}}(L) = \mathcal{M}_{f_{\mathcal{D}}}(K_n)$. It is easy to see that if $\mathcal{M}_{f_{\mathcal{D}}}(L) = \mathcal{M}_{f_{\mathcal{D}}}(K_n)$, then the graph L is uniquely determined, that is, L is isomorphic to K_n. It is thus proved that $B_3(K_n) \le n-1$.

Finally, we show that $B_3(K_n) = n-1$. Suppose that $B_3(K_n) = k < n-1$. By Proposition 1, there exists a k-edge-coloring f of K_n with $k < n-1$. By the assumptions, the edge-coloring f provides a pot $\mathcal{T}_f$ satisfying Lemma 1. For every $v \in V(K_n)$, at least one color of f appears twice in the multi-palette $P_f(v)$, since $k < n-1$. Moreover, there exist at least two vertices $u, v \in V(K_n)$ such that $P_f(u)$, $P_f(v)$ contain the same color a more than once. Hence, there exist uu_1, uu_2, $vv_1, vv_2 \in E(K_n)$ such that $f(uu_1) = f(uu_2) = f(vv_1) = f(vv_2) = a$. By property (iii) of Lemma 1, the vertex u_1 is not adjacent to v, a contradiction. It is thus proved that $B_3(K_n) = n-1$. □

Corollary 6.

$$B_3(K_{m,n}) = \min(m, n).$$

Proof. Without loss of generality, we can assume that $m \leq n$. We use Proposition 6 to find a pot $\mathcal{T}_{f_\mathcal{D}}$ realizing the graph $K_{m,n}$ and no graph of order smaller than $m+n$. The graph $K_{m,n}$ has a decomposition $\mathcal{D}$ into the subgraphs H_i, $1 \leq i \leq m$, where each H_i is the star $K_{1,n}$. We color the subgraphs H_i by disjoint color-sets $\mathcal{C}_{H_i} = \{a_i\}$ and consider the edge-coloring f_{H_i} that colors each edge of H_i by a_i. The edge-coloring f_{H_i} defines the pot $\mathcal{T}_{f_{H_i}} = \{\{a_i^n\}, \{\hat{a}_i\}\}$ and $\mathcal{M}_{f_{H_i}}(K_{1,n}) = \{\{a_i^n\}^1, \{\hat{a}_i\}^n\}$. Combining the pots $\mathcal{T}_{f_{H_i}}$, we obtain the pot $\mathcal{T}_{f_\mathcal{D}} = \{\{\hat{a}_1, \hat{a}_2, \ldots, \hat{a}_m\}, \{a_i^n\} : 1 \leq i \leq m\}$ realizing the graph $K_{m,n}$ and $\mathcal{M}_f(K_{m,n}) = \{\{\hat{a}_1, \hat{a}_2, \ldots, \hat{a}_m\}^n, \{a_i^n\}^1 : 1 \leq i \leq m\}$.

Set $\mathcal{D}^* = \mathcal{D}$ and $\mathcal{T}^* = \{\{\hat{a}_1\}, \{a_i^n\} : 1 \leq i \leq m\}$. The elements of $\mathcal{T}_{f_\mathcal{D}}$ can be partitioned into the following subsets A_t, $t \in \mathcal{T}^*$: $A_{\{\hat{a}_1\}} = \{\{\hat{a}_1, \hat{a}_2, \ldots, \hat{a}_m\}\}$; $A_{\{a_i^n\}} = \{\{a_i^n\}\}$, for $1 \leq i \leq m$. It is easy to see that no element of $\mathcal{T}_{f_\mathcal{D}}$ can belong to more than one subset A_t, that is, property (0) of Proposition 6 is satisfied. For every $H_i \in \mathcal{D}$, if L_{H_i} is a graph that can be constructed from $\mathcal{T}_{f_{H_i}}$, then $\mathcal{M}_{f_{H_i}}(L_{H_i})$ contains $\lambda_{H_i} \geq 1$ copies of $\mathcal{M}_{f_{H_i}}(K_{1,n})$. The property follows from the fact that the number of half-edges that are labeled by a_i is equal to the number of half-edges that are labeled by $\hat{a}_i$, since L_{H_i} is a complete complex. Hence, property (1) of Proposition 6 is satisfied. Since Proposition 6 holds, the pot $\mathcal{T}_{f_\mathcal{D}}$ realizes no graph of order smaller than $m+n$.

We now show that if the graph has order $m+n$, then it is isomorphic to the graph $K_{m,n}$. If L is a graph that can be constructed from $\mathcal{T}_{f_\mathcal{D}}$, then $\mathcal{M}_{f_\mathcal{D}}(L) = \{\{\hat{a}_1, \hat{a}_2, \ldots, \hat{a}_m\}^{m_0}, \{a_i^n\}^{m_i}\colon m_0, m_i \geq 0, 1 \leq i \leq m\}$ and the following equalities hold: $n \cdot m_i = m_0$ and $|V(L)| = \sum_{i=0}^{m} m_i = (n+m)m_i > 0$, for every $1 \leq i \leq m$. Therefore, $|V(L)| = m+n$ if and only if $m_i = 1$ for every $1 \leq i \leq m$, that is, if and only if $\mathcal{M}_{f_\mathcal{D}}(L) = \mathcal{M}_{f_\mathcal{D}}(K_{m,n})$. It is easy to see that if $\mathcal{M}_{f_\mathcal{D}}(L) = \mathcal{M}_{f_\mathcal{D}}(K_{m,n})$, then the graph L is uniquely determined, that is, L is isomorphic to $K_{m,n}$. It is thus proved that $\mathcal{T}_{f_\mathcal{D}}$ realizes the graph $K_{m,n}$ and satisfies the conditions in Scenario 3, whence $B_3(K_{m,n}) \leq m$.

Finally, we show that $B_3(K_{m,n}) = m$. Suppose that $B_3(K_{m,n}) = k < m \leq n$. By Proposition 1, there exists a k-edge-coloring f of $K_{m,n}$. Let $U \cup W$ be the bipartition of $K_{m,n}$. For every $u \in U$, at least one color of f appears twice in the multi-palette $P_f(u)$, since every vertex of U has degree $n > k$. Moreover, there exist at least two vertices $u, v \in U$ such that $P_f(u)$, $P_f(v)$ contain the same color a more than once, since $|U| = m > k$. Hence, there exist uu_1, uu_2, $vv_1, vv_2 \in E(K_{m,n})$ such that $f(uu_1) = f(uu_2) = f(vv_1) = f(vv_2) = a$. By property *(iii)* of Lemma 1, the vertex u is not adjacent to v_1, a contradiction. It is thus proved that $B_3(K_{m,n}) = m$. □

4.1 Bounds from cycle decompositions

We construct pots from cycle decompositions, that is decompositions into cycles, providing upper bounds for $B_3(G)$. Cycle decompositions are extensively studied – see the survey papers [2] and [15]– and our results can be viewed as an application of cycle decompositions to the self-assembly of DNA structures. It is known that every Eulerian graph has a cycle decomposition [20]. The structure of a cycle allows the definition of a pot realizing a cycle and having "nice" properties (see Lemma 2). Given a cycle decomposition $\mathcal{D}$ of an Eulerian graph G, by the properties in Lemma 2, we can find a pot $\mathcal{T}_{f_{\mathcal{D}}}$ realizing the graph G and satisfying the conditions in Scenario 3 (see Proposition 7); we can thus find an upper bound for $B_3(G)$. In Proposition 8, non-Eulerian graphs are considered.

Lemma 2. *Let $C_n = (v_1, v_2, \ldots, v_n, v_1)$ be a cycle of length $n \geq 3$. Let $\overline{f}$ be the edge-coloring of C_n with color-set $\{a_i : 1 \leq i \leq n-1\}$ such that $\overline{f}(v_iv_{i+1}) = a_i$ for $1 \leq i \leq n-1$ and $\overline{f}(v_1v_n) = a_1$. The edge-coloring $\overline{f}$ defines the pot $\mathcal{T}_{\overline{f}} = \{\bar{t}_i : 0 \leq i \leq n-1\}$, where $\bar{t}_0 = \{a_1^2\}$, $\bar{t}_{n-1} = \{\hat{a}_1, \hat{a}_{n-1}\}$ and $\bar{t}_i = \{\hat{a}_i, a_{i+1}\}$ for $1 \leq i \leq n-2$.*

The pot $\mathcal{T}_{\overline{f}}$ realizes the graph C_n and satisfies the conditions in Scenario 3. The multiset $\mathcal{M}_{\overline{f}}(L)$ of a graph L that can be constructed from $\mathcal{T}_{\overline{f}}$ contains $\lambda \geq 1$ copies of $\mathcal{M}_{\overline{f}}(C_n) = \{\bar{t}_i^1 : 1 \leq i \leq n-1\}$. Moreover, if L is isomorphic to C_n, then for every $0 \leq i \leq n-1$ there exists exactly one edge $uv \in E(L)$ such that $\{t_{\overline{f}}(u), t_{\overline{f}}(v)\} = \{\bar{t}_i, \bar{t}_{i+1}\}$, where the subscripts are considered modulo n.

Proof. Notice that for every $0 \leq i \leq n-1$ there exists exactly one vertex of C_n whose tile type with respect to $\overline{f}$ is $\bar{t}_i$, that is, $\mathcal{M}_{\overline{f}}(C_n) = \{\bar{t}_i^1 : 0 \leq i \leq n-1\}$. Let L be a graph that can be constructed from $\mathcal{T}_{\overline{f}}$. We set $\mathcal{M}_{\overline{f}}(L) = \{\bar{t}_i^{m_i} : m_i \geq 0, 0 \leq i \leq n-1\}$ and show that $\mathcal{M}_{\overline{f}}(L)$ contains $\lambda \geq 1$ copies of $\mathcal{M}_{\overline{f}}(C_n)$. For every $1 \leq i \leq n-1$, the number of half-edges that are labeled by a_i is equal to the number of half-edges that are labeled by $\hat{a}_i$, since L is a complete complex. Consequently, the following equalities hold: $2m_0 = m_1 + m_{n-1}$ and $m_{i-1} = m_i$ for every $2 \leq i \leq n-1$. Whence $m_1 = m_2 = \cdots = m_{n-1}$ and $m_0 = m_1$, that is, $\mathcal{M}_{\overline{f}}(L)$ contains $\lambda = m_1 \geq 1$ copies of $\mathcal{M}_{\overline{f}}(C_n)$. Thus $|V(L)| \geq |V(C_n)|$; in particular, $|V(L)| = n$ if and only if $\mathcal{M}_{\overline{f}}(L) = \mathcal{M}_{\overline{f}}(C_n)$. In this case, notice that a vertex of L having tile type $\bar{t}_i$ with respect to $\overline{f}$ is adjacent to two vertices, one with tile type $\bar{t}_{i-1}$ and the other with tile type $\bar{t}_{i+1}$ with respect to $\overline{f}$. Hence, the graph L is isomorphic to C_n provided that $\mathcal{M}_{\overline{f}}(L) = \mathcal{M}_{\overline{f}}(C_n)$. Thus $\mathcal{T}_{\overline{f}}$ realizes the graph C_n and satisfies the conditions in Scenario 3. It also follows that for every $0 \leq i \leq n-1$ there exists exactly one edge $uv \in E(L)$ such that $\{t_{\overline{f}}(u), t_{\overline{f}}(v)\} = \{\bar{t}_i, \bar{t}_{i+1}\}$, where the subscripts are considered modulo n. $\square$

Let $f : E(G) \to \mathcal{C}$, $f' : E(G) \to \mathcal{C}'$ be edge-colorings of the graph G. We say that f and f' are *equivalent* if there exists a bijection $\pi : \mathcal{C} \to \mathcal{C}'$ such that $f'(e) = \pi(f(e))$ for every $e \in E(G)$. Equivalent edge-colorings f, f' define equivalent pots, as we are going to explain. We say that the pots $\mathcal{T}_f$, $\mathcal{T}_{f'}$ associated to f, f', respectively, are *equivalent* if $\mathcal{T}_{f'}$ can be obtained from $\mathcal{T}_f$ by replacing, in every $t \in \mathcal{T}_f$, each label a (respectively, $\hat{a}$) coming from the color-set $\mathcal{C}$ with the label $\pi(a)$ (respectively, $\widehat{\pi(a)}$) coming from the color-set $\mathcal{C}'$. Accordingly, a tile type $t' \in \mathcal{T}_{f'}$ is equivalent to the tile type $t \in \mathcal{T}_f$ if t' is obtained from t by replacing the labels in t as described above.

Proposition 7. *Let G be an Eulerian graph and let $\mathcal{D}$ be a cycle decomposition of G. For every cycle $H \in \mathcal{D}$ of length $n_H \geq 3$, we consider an edge-coloring f_H and the associated pot $\mathcal{T}_{f_H}$ that are equivalent to the edge-coloring $\overline{f}$ and to the associated pot $\mathcal{T}_{\overline{f}}$, respectively, of the cycle C_{n_H} in Lemma 2. Let $f_{\mathcal{D}}$ be the edge-coloring of G obtained by combining the edge-colorings f_H and let $\mathcal{T}_{f_{\mathcal{D}}}$ be the associated pot obtained by combining the pots $\mathcal{T}_{f_H}$.*

The pot $\mathcal{T}_{f_{\mathcal{D}}} = \{t_j : 1 \leq j \leq |V(G)|\}$ realizes the graph G and satisfies the conditions in Scenario 3. Whence $B_3(G) \leq |E(G)| - |\mathcal{D}|$.

Proof. We note that $|\mathcal{T}_{f_{\mathcal{D}}}| = |V(G)|$ and, consequently, $\mathcal{M}_{f_{\mathcal{D}}}(G) = \{t_j^1 : 1 \leq j \leq |V(G)|\}$. It follows from the fact that G is the edge-disjoint union of the graphs $H \in \mathcal{D}$ that are colored by disjoint color-sets and $\mathcal{M}_{f_H}(H) = \{t^1 : t \in \mathcal{T}_{f_H}\}$, since Lemma 2 holds. Observe that every $t \in \mathcal{T}_{f_H}$ is contained in exactly one element $t_j \in \mathcal{T}_{f_{\mathcal{D}}}$.

Let L be a graph that can be constructed from the pot $\mathcal{T}_{f_{\mathcal{D}}}$. We set $\mathcal{M}_{f_{\mathcal{D}}}(L) = \{t_j^{m_j} : m_j \geq 0, 1 \leq j \leq |V(G)|\}$ and prove that $|V(L)| \geq |V(G)|$. For every $H \in \mathcal{D}$, we denote by L_H the subgraph of L induced by the color-set $\mathcal{C}_H$ (the color-set of f_H). Since the graphs $H \in \mathcal{D}$ are colored by disjoint color-sets, the graph L is the edge-disjoint union of the graphs L_H. As proved in Proposition 6, L_H is non-empty for every $H \in \mathcal{D}$. A graph L_H is constructed from the pot $\mathcal{T}_{f_H}$. By Lemma 2, the multiset $\mathcal{M}_{f_H}(L_H)$ contains $\lambda_H \geq 1$ copies of $\mathcal{M}_{f_H}(H)$, that is, for every tile type $t \in \mathcal{T}_{f_H}$ there exists at least one vertex of L_H having tile type t with respect to f_H. Since $V(L_H) \subseteq V(L)$ and every $t \in \mathcal{T}_{f_H}$ is contained in exactly one element $t_j \in \mathcal{T}_{f_{\mathcal{D}}}$, we have $m_j \geq 1$ for every $1 \leq j \leq |V(G)|$. Hence $|V(L)| = \sum_{j=1}^{|V(G)|} m_j \geq |V(G)|$. In particular, $|V(L)| = |V(G)|$ if and only if $m_j = 1$ for every $1 \leq j \leq |V(G)|$, that is, $\mathcal{M}_{f_{\mathcal{D}}}(L) = \mathcal{M}_{f_{\mathcal{D}}}(G)$.

We show that if $\mathcal{M}_{f_{\mathcal{D}}}(L) = \mathcal{M}_{f_{\mathcal{D}}}(G)$, then L is isomorphic to G. Firstly, notice that every edge $uv \in E(G)$ is contained in exactly one cycle $H \in \mathcal{D}$ and since Lemma 2 holds, there exists exactly one integer $0 \leq i \leq n_H - 1$ such that the set $\{t_{f_H}(u), t_{f_H}(v)\}$ is equivalent to $\{\overline{t}_i, \overline{t}_{i+1}\}$, that is, $t_{f_H}(u)$ is equivalent to $\overline{t}_i$ and $t_{f_H}(v)$ is equivalent to $\overline{t}_{i+1}$ or vice versa. For the sake of brevity, we say that the edge $uv \in E(G)$ has form $\{\overline{t}_i, \overline{t}_{i+1}\}$ with respect to f_H. Since $\mathcal{M}_{f_\mathcal{D}}(L) = \mathcal{M}_{f_\mathcal{D}}(G)$ implies $\mathcal{M}_{f_H}(L_H) = \mathcal{M}_{f_H}(H)$, and so L_H is isomorphic to H, we can repeat the same observation for L.

Let θ be the correspondence between $V(G)$ and $V(L)$ that maps the vertex $v \in V(G)$ to the vertex $\theta(v) \in V(L)$ such that $t_{f_\mathcal{D}}(v) = t_{f_\mathcal{D}}(\theta(v))$. Let φ be the correspondence between $E(G)$ and $E(L)$ that maps the edge $uv \in E(G)$ having form $\{\bar{t}_i, \bar{t}_{i+1}\}$ with respect to f_H to the edge $\varphi(uv)$ having the same form as uv with respect to f_H. We prove that the pair (θ, φ) is an isomorphism between G and L. The correspondence θ is a bijection between $V(G)$ and $V(L)$, since $\mathcal{M}_{f_\mathcal{D}}(G) = \mathcal{M}_{f_\mathcal{D}}(L)$ and for every $t_j \in \mathcal{T}_{f_\mathcal{D}}$ there exists exactly one vertex $v \in V(G)$ and exactly one vertex $v' \in V(L)$ such that $t_{f_\mathcal{D}}(v) = t_{f_\mathcal{D}}(v') = t_j$. The correspondence φ is a bijection between $E(G)$ and $E(L)$, since for every $H \in \mathcal{D}$ and $0 \le i \le n_H - 1$ there exists exactly one edge $uv \in E(G)$ and exactly one edge $u'v' \in E(L)$ having form $\{\bar{t}_i, \bar{t}_{i+1}\}$ with respect to f_H, as Lemma 2 holds. We show that $\varphi(uv) = \theta(u)\theta(v)$ for every $uv \in E(G)$. As remarked, an edge $uv \in E(G)$ has form $\{\bar{t}_i, \bar{t}_{i+1}\}$ with respect to f_H, where H is the cycle of $\mathcal{D}$ such that $uv \in E(H)$ and i is a suitable integer $0 \le i \le n_H - 1$. Without loss of generality, we can assume that $t_{f_H}(u)$ is equivalent to $\bar{t}_i$ and $t_{f_H}(v)$ is equivalent to $\bar{t}_{i+1}$. By definition of φ, the edge $\varphi(uv) \in E(L)$ has form $\{\bar{t}_i, \bar{t}_{i+1}\}$ with respect to f_H. Set $t_{f_\mathcal{D}}(u) = t_r \in \mathcal{T}_{f_\mathcal{D}}$ and $t_{f_\mathcal{D}}(v) = t_s \in \mathcal{T}_{f_\mathcal{D}}$. By definition of θ, we have $t_{f_\mathcal{D}}(\theta(u)) = t_r$ and $t_{f_\mathcal{D}}(\theta(v)) = t_s$. Since t_r and t_s contain $t_{f_H}(u)$ and $t_{f_H}(v)$, respectively, which are equivalent to $\bar{t}_i$ and $\bar{t}_{i+1}$, respectively, the edge $\theta(u)\theta(v) \in E(L_H)$ has form $\{\bar{t}_i, \bar{t}_{i+1}\}$ with respect to f_H. By Lemma 2, the graph L_H has exactly one edge having form $\{\bar{t}_i, \bar{t}_{i+1}\}$ with respect to f_H. Consequently, the graph L has exactly one edge having form $\{\bar{t}_i, \bar{t}_{i+1}\}$ with respect to f_H. Whence $\varphi(uv) = \theta(u)\theta(v)$. It is thus proved that $\mathcal{T}_{f_\mathcal{D}}$ realizes the graph G and satisfies the conditions in Scenario 3. It also follows that $B_3(G) \le \sum_{H \in \mathcal{D}} |\mathcal{C}_H|$, where $|\mathcal{C}_H| = n_H - 1$, since Lemma 2 holds. Whence $B_3(G) \le \sum_{H \in \mathcal{D}} (n_H - 1) = |E(G)| - |\mathcal{D}|$, since $|E(G)| = \sum_{H \in \mathcal{D}} |E(H)| = \sum_{H \in \mathcal{D}} n_H$. The assertion follows. □

Proposition 8. *Let G be a connected graph having $2\ell > 0$ vertices of odd degree. The graph G has a decomposition $\mathcal{D}$ into cycles (possibly none) and ℓ paths connecting vertices of odd degree. Then $B_3(G) \le |E(G)| - |\mathcal{D}| + \ell$.*

Proof. Firstly, we define an edge-coloring f^* and the associated pot $\mathcal{T}_{f^*}$ realizing paths. Given a cycle $C_{n+2} = (v_1, v_2, \ldots, v_{n+2}, v_1)$ which is colored by the edge-coloring $\overline{f}$ in Lemma 2, we denote by f^* the restriction of $\overline{f}$ to the edges of the path $P_n = (v_2, \ldots, v_{n+2})$. Notice that f^* has color-set $\{a_2, \ldots, a_{n+1}\}$. Let $\mathcal{T}_{f^*} = \{t_i^* : 1 \le i \le n+1\}$ be the pot associated to f^* that can be obtained from the pot $\mathcal{T}_{\overline{f}}$ in Lemma 2 as follows: $t_1^* = \bar{t}_1 \smallsetminus \{\hat{a}_1\} = \{a_2\}$; $t_{n+1}^* = \bar{t}_{n+1} \smallsetminus \{\hat{a}_1\} = \{\hat{a}_{n+1}\}$; $t_i^* = \bar{t}_i$ for $2 \le i \le n$. The pot $\mathcal{T}_{f^*}$ inherits the same properties as $\mathcal{T}_{\overline{f}}$. More specifically, it realizes the graph P_n and satisfies the conditions in Scenario 3; if L is a graph that can be constructed from $\mathcal{T}_{f^*}$ then $\mathcal{M}_{f^*}(L)$ contains $\lambda \geq 1$ copies of $\mathcal{M}_{f^*}(P_n)$; if L is isomorphic to P_n, then for every $1 \leq i \leq n$ the graph L contains exactly one edge uv such that $\{t_{f^*}(u), t_{f^*}(v)\} = \{t_i^*, t_{i+1}^*\}$.

We show that G has a decomposition $\mathcal{D}$ into cycles and paths. Let G_1 be the graph obtained by connecting the vertices of odd degree in G to a vertex u not belonging to $V(G)$. Since G_1 is Eulerian, it has a cycle decomposition $\mathcal{D}_1$. Let $\mathcal{D}$ be the decomposition of G obtained from $\mathcal{D}_1$ by deleting the vertex u into the cycles of $\mathcal{D}_1$ containing it. The decompositions $\mathcal{D}$ consists of cycles and ℓ paths connecting the vertices of odd degree in G.

We use $\mathcal{D}$ to define a pot $\mathcal{T}_{f_\mathcal{D}}$. We color the elements of $\mathcal{D}$ by disjoint color-sets. For every cycle $H \in \mathcal{D}$ we consider the edge-coloring f_H and the associated pot $\mathcal{T}_{f_H}$ that are equivalent to $\overline{f}$ and $\mathcal{T}_{\overline{f}}$, respectively, in Lemma 2. For every path $H \in \mathcal{D}$ we consider the edge-coloring f_H and the associated pot $\mathcal{T}_{f_H}$ that are equivalent to the edge-coloring f^* and $\mathcal{T}_{f^*}$, respectively. Let $f_\mathcal{D}$ be the edge-coloring of G obtained by combining the edge-colorings f_H and let $\mathcal{T}_{f_\mathcal{D}}$ be the associated pot obtained by combining the pots $\mathcal{T}_{f_H}$. Since $\mathcal{T}_{f^*}$ inherits the same properties as $\mathcal{T}_{\overline{f}}$, we can repeat the proof of Proposition 7 and prove that $\mathcal{T}_{f_\mathcal{D}}$ realizes the graph G and satisfies the conditions in Scenario 3. Whence $B_3(G) \leq \sum_{H \in \mathcal{D}} |\mathcal{C}_H|$. Notice that $|\mathcal{C}_H| = n_H - 1$ if $H \in \mathcal{D}$ is a cycle of length n_H; $|\mathcal{C}_H| = n_H$ if $H \in \mathcal{D}$ is a path with n_H edges. Moreover, $|E(G)| = \sum_{H \in \mathcal{D}} |E(H)| = \sum_{H \in \mathcal{D}} n_H$. Therefore $B_3(G) \leq |E(G)| - |\mathcal{D}| + \ell$. □

Proposition 8 can be applied to a tree, in this case the decomposition contains no cycle. Unlike Proposition 6, where a decomposition contains arbitrary subgraphs, that ones in Proposition 7 and 8 consist of prescribed graphs (cycles). The provided upper bounds suggest to select the decompositions with the maximum possible number of cycles.

5 Conclusion

We provide a strategy for computing the minimum number of bond-edge types and tile types needed in the construction of any target graph. Our techniques allow to efficiently construct the target graph by avoiding the assembly of undesired graphs as described in Scenario 2 and 3. We also describe the problem on DNA self-assembly from a new graph theoretic perspective employing edge-colorings and graph decompositions. We emphasize that although we are motivated by DNA self-assembly, the combinatorial tools and methods presented may apply to other form of assembly whose building blocks bond to each other according to certain criteria. That might be the case for pathway reconstruction on 3D NMR maps, where edge-colored paths whose edges follow a predefined order of colors are considered – see for instance [19].

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