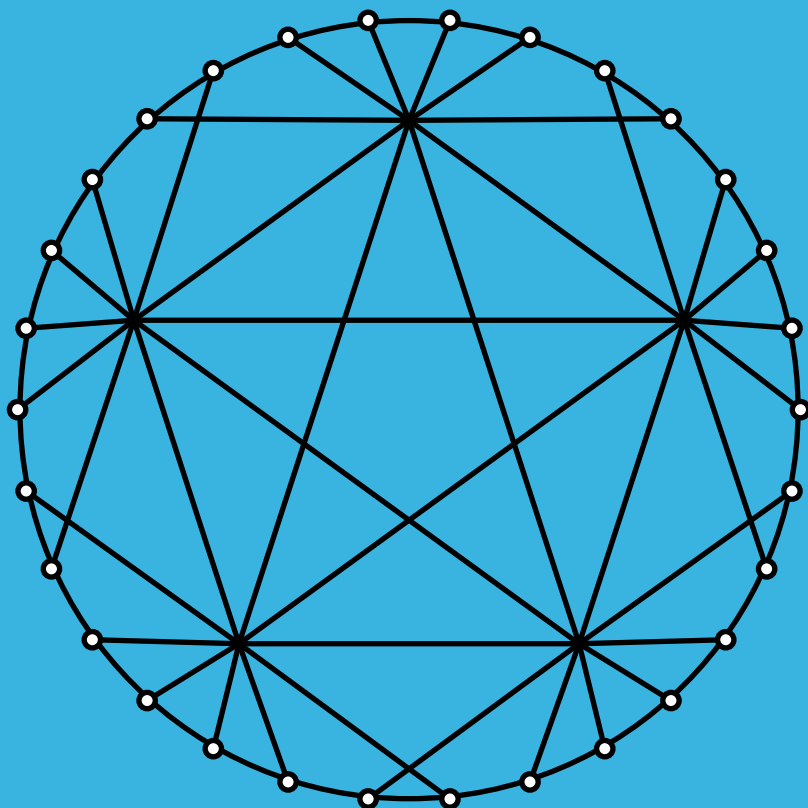


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On non-isomorphic biminimal pots realizing the cube

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Abstract. This paper deals with two new graph invariants called the minimum number of tile types and the minimum number of bond-edge types, which have been introduced to study DNA self-assembly processes. In particular, we disprove a conjecture recently proposed in [L. Almodóvar et al., Computational complexity and pragmatic solutions for flexible tile based DNA self-assembly, <https://arxiv.org/abs/2108.00035>] on the non-existence of biminimal pots realizing the cube, namely pots simultaneously achieving both minimums. Indeed, after introducing the concepts of isomorphic pots and isomorphic realizations, we present two biminimal pots realizing the cube and show that these two pots are unique up to isomorphism.

1 Introduction

In this paper we study two new graph invariants, namely the minimum number of tile types and the minimum number of bond-edge types. These two parameters have been introduced to optimally build a target graph-like structure through DNA self-assembly processes using branched junction molecules [8]. We refer the reader to [6, 11, 14] for experimental works on tile-based DNA self-assembly and to [7] for an overview of mathematical problems arising from these processes. In this context, the minimum number of tile types corresponds to the smallest number of molecules required to self-assemble a larger molecule with the structure of a target graph G ;

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the minimum number of bond-edge types represents instead the smallest number of bonds needed to construct G . The increasing interest in these parameters is reflected in the growing body of work addressing their computation for certain classes of graphs under different experimental conditions [1, 2, 3, 4, 8, 9, 10, 12]. Except for [9], in all these studies it is assumed that the molecules have “flexible” arms, so that no geometric properties have to be encoded into the mathematical formalism.

Here, we focus on a conjecture about the assembly of the cube Q posed in [1]. In this recent paper, Almodóvar et al. concentrate on determining an optimal set of molecules, called *pot*, that self-assembles into the cube Q so that no graph with order smaller than that of Q , or having the same order but not isomorphic to Q , can be constructed. More precisely, the authors provide two distinct pots assembling the cube in this scenario: one pot utilizes the minimum number of tile types, which equals 6, and the other utilizes the minimum number of bond-edge types, which is 5. They conjecture that there is no pot achieving both the minimum number of tile types *and* the minimum number of bond-edge types for the cube Q . In this work, we disprove this conjecture by presenting two *biminimal* pots assembling the cube and having 6 tile types and 5 bond-edge types. Importantly, we show that these two pots are unique (up to isomorphism). To this end, we use edge-colorings and orientations of an undirected graph G to describe the problem of computing the minimum number of tile types and the minimum number of bond-edge types of G . Note that these notions have already been employed to study the two quantities of interest; see [8] and [4] where, in the latter, this topic is strongly related to graph decompositions [5] and some chromatic parameters. Nonetheless, we believe our setup facilitates the mathematical exposition of the theoretical results while offering another avenue to study the minimum number of tile types and the minimum number of bond-edge types of a graph G (for instance, via weighted graphs).

This paper is organized as follows. In Section 2, we introduce the background definitions and basic properties used in this work. In Section 3, we recall known results related to the assembly of the cube. In Section 4, we show that there are only two biminimal pots (up to isomorphism) that assemble the cube in the considered setting.

2 Preliminaries

In this paper, graphs are connected and may have loops or multiple edges. To avoid ambiguity, we define a graph G as a triple $(V(G), E(G), \mu)$ where $V(G)$ is the set of vertices, $E(G)$ is the set of edges, and $\mu : E(G) \rightarrow V(G)^{(2)}$ is a map, where

1. $V(G)^{(2)} = V(G) \times V(G)$, and in this case G is *directed*; or
2. $V(G)^{(2)}$ is the set of (not necessarily distinct) unordered pairs of vertices of G , and in this case G is *undirected*.

If $\mu(e) = \{x, y\}$ or $\mu(e) = (x, y)$, then x and y are called the end-vertices of e . We will sometimes identify the edge e with $\mu(e)$ and write $e = \mu(e)$. Let $L(G)$ denote the set of all loops of G and, given a vertex x of G , we denote by G_x the subgraph of G induced by all the edges (including loops) of G incident with x .

An *edge-coloring* of G with c colors is a map $\lambda : E(G) \rightarrow [1, c]$, where $[1, c]$ denotes the set of all positive integers not greater than c . The set $\lambda^{-1}(j)$ of all edges colored j is referred to as the j -color class. Clearly, the color classes of G partition between them $E(G)$, hence $|E(G)| = \sum_{j=1}^c |\lambda^{-1}(j)|$.

A *tile* is a finite multiset of \mathbb{Z} and a finite set of tiles is called a *pot*. Given a pot P , we denote by $\Sigma(P) \subset \mathbb{N}$ the set of all distinct positive integers (colors), say c_1, \dots, c_n , such that c_i or $-c_i$ appears in some tile of P , for every $i \in [1, n]$. In the following, we define the concepts of tile and pot induced by an edge-coloring λ .

1. The tile induced by λ on $x \in V(G)$ is the multiset

$$\tau_x(\lambda) = \{e_x \lambda(e) \mid e \in E(G_x)\} \cup \{\lambda(e) \mid e \in L(G_x)\} \text{ where}$$

$$e_x = \begin{cases} 1 & \text{if } e = \{x, y\}, \text{ or } e = (x, y) \text{ and } x \neq y, \\ -1 & \text{if } e = (y, x). \end{cases}$$

2. The pot induced by λ (on G) is the set $\mathcal{P}(\lambda) = \{\tau_x(\lambda) \mid x \in V(G)\}$ of distinct tiles induced by λ .

We note that the concept of tile given above coincides with the equivalent notion of *tile type* used in previous works on this topic, as in [7, 8]. We also

recall that for an edge-coloring λ of an undirected graph G , the notion of tile $\tau_x(\lambda)$ on $x \in V(G)$ coincides with the notion of multi-palette of x with respect to λ (see [4]). In the following we will denote multisets using the right exponential notation, for instance by $X = \{1^2, 2\}$ we will mean that 1 appears twice, while 2 appears exactly once in X .

Example 2.1. Let G be the directed graph in Figure 1 and $\lambda : E(G) \rightarrow [1, 3]$ the associated edge-coloring. The tiles induced by λ are: $\tau_{x_0}(\lambda) = \{1, 2^2\}$, $\tau_{x_1}(\lambda) = \{-1, -2, 3\}$, $\tau_{x_2}(\lambda) = \{1, -2, -3\}$, $\tau_{x_3}(\lambda) = \{1, -1^2\}$. Hence the set

$$\mathcal{P}(\lambda) = \{\{1, 2^2\}, \{-1, -2, 3\}, \{1, -2, -3\}, \{1, -1^2\}\}$$

is the pot induced by λ on G .

Example 2.2. Let G_1 be the directed graph in Figure 2 and $\lambda_1 : E(G_1) \rightarrow [1, 3]$ the associated edge-coloring. Note that the pot induced by λ_1 is nothing but the pot $\mathcal{P}(\lambda)$ of Example 2.1.

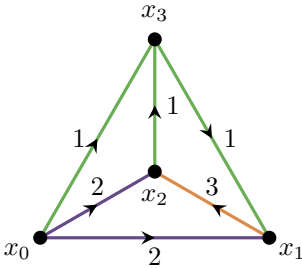


Figure 1.

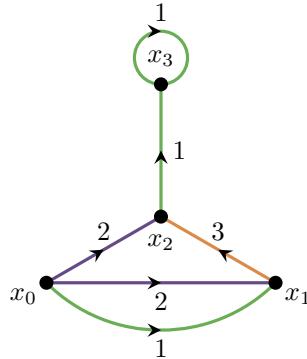


Figure 2.

From now on, G denotes an undirected graph. Also, by $Or(G)$ we mean the set of all *orientations* of G , that is, all directed graphs obtained from G by choosing an orientation of its edges. We denote an arbitrary graph in $Or(G)$ by \vec{G} , and for every edge $e \in E(G)$, by \vec{e} and \bar{e} we mean the two orientations of e . Note that for a loop, the two orientations coincide.

We recall here the standard terminology and notation used for some undirected graphs, see for instance [15]. The *degree* of a vertex x of a simple graph G is the number of vertices of G adjacent to x . If every vertex of G has degree r , one says that G is r -regular. In particular, a 3-regular graph, is also called a *cubic* graph. A set of pairwise non-adjacent vertices of a graph G is called *independent*. A graph G is called *bipartite* if $V(G)$ has a bipartition into two independent subsets. We denote by $C = (x_1, \dots, x_k)$ the *cycle*

C of length k whose edges are $\{x_1, x_2\}, \dots, \{x_{k-1}, x_k\}, \{x_k, x_{k+1} = x_1\}$. We denote by $[x_1, \dots, x_k]$ the *path* with k vertices (and length $k - 1$) obtained from C by removing the edge $\{x_1, x_k\}$. We recall that a graph is bipartite if and only if it contains no cycle of odd length. A *star* of size k (a k -star) is a set of k edges, none of which are loops, all incident in the same vertex. Clearly, a 2-star is nothing but a path of length 2. A *matching* of a graph G is a set of pairwise non-incident edges of G , none of which are loops.

Let $\lambda : E(\vec{G}) \rightarrow [1, c]$ be an edge-coloring of an orientation of G . The edge-coloring $\underline{\lambda}$ of G induced by λ is defined as follows: if $\vec{e} \in E(\vec{G})$ is an orientation of $e \in E(G)$, then $\underline{\lambda}(e) = \lambda(\vec{e})$. Given two orientations \vec{G}_1 and \vec{G}_2 of G , the map $\sigma : E(\vec{G}_1) \rightarrow E(\vec{G}_2)$ such that $\sigma(\vec{e}) \in \{\vec{e}, \bar{\vec{e}}\}$ is called the *orientation map* from \vec{G}_1 to \vec{G}_2 . Clearly, σ^{-1} is an orientation map, as well.

Given a map f defined on a set $X \subseteq \mathbb{Z}$, we extend f pointwise to any (family of) multisets of X . For example, letting $\|z\|$ denote the absolute value of $z \in \mathbb{Z}$, and given the tile $t = \{z_i^{\mu_i} \mid i = 1, \dots, u\}$ containing exactly μ_i copies of z_i for each i , then $\|t\| = \{\|z_i\|^{\mu_i} \mid i = 1, \dots, u\}$.

The following result points out a clear connection between tiles and pots of λ and $\underline{\lambda}$. Its proof is straightforward and therefore left to the reader. Note that this inequality was also obtained in [4].

Lemma 2.3. $\tau_x(\underline{\lambda}) = \|\tau_x(\lambda)\|$ and $\mathcal{P}(\underline{\lambda}) = \|\mathcal{P}(\lambda)\|$. Therefore, $|\mathcal{P}(\underline{\lambda})| \leq |\mathcal{P}(\lambda)|$.

Definition 2.4. Let G be an undirected graph and let P be a pot. A realization of G through P is an edge-coloring λ of an orientation \vec{G} of G such that $\mathcal{P}(\lambda) \subseteq P$. In this case, we say that P realizes G and write $G \in \mathcal{O}(P)$ (meaning that G is in the output of P).

Furthermore, we say that P realizes G in Scenario $i \in [1, 3]$, and write $G \in \mathcal{O}_i(P)$, if the following conditions hold:

$i = 1$: $G \in \mathcal{O}(P)$.

$i = 2$: $G \in \mathcal{O}(P)$ and there is no $H \in \mathcal{O}(P)$ such that $|V(H)| < |V(G)|$.

$i = 3$: $G \in \mathcal{O}(P)$ and there is no $H \in \mathcal{O}(P)$ such that $H \not\cong G$ and $|V(H)| \leq |V(G)|$.

If $G \in \mathcal{O}_i(P)$, we say that P i -realizes G , or that there exists an i -realization of G through P .

The minimum size of a pot i -realizing G is denoted by

$$T_i(G) = \min\{|P| \mid P \text{ is a pot that } i\text{-realizes } G\}.$$

The minimum number of colors used by a pot that i -realizes G is denoted by

$$B_i(G) = \min\{|\Sigma(P)| \mid P \text{ is a pot that } i\text{-realizes } G\}.$$

These parameters are called *minimum number of tiles* (or, equivalently, of tile types) and *minimum number of bond-edge types*, respectively. For $i \in [1, 3]$, $T_i(G)$ and $B_i(G)$ have been determined for cycles, trees, complete and complete bipartite graphs in [8]. Recent works have instead focused on Platonic solids, square and triangular lattices, and other graph classes [1, 2, 3, 10, 12].

Definition 2.5. A pot P that i -realizes G is *biminimal* if $|P| = T_i(G)$ and $|\Sigma(P)| = B_i(G)$.

We now introduce the concept of isomorphic pots.

Definition 2.6. Two pots P and P' are *isomorphic* if there exists a bijection (isomorphism) $f : \Sigma(P) \cup -\Sigma(P) \rightarrow \Sigma(P') \cup -\Sigma(P')$ such that $f(-i) = -f(i)$ and $f(P) = P'$.

Clearly, isomorphic pots have the same cardinality and use the same number of colors. Given two isomorphic pots P and P' , we denote by $f^+ : \Sigma(P) \rightarrow \Sigma(P')$ the map defined as follows: $f^+(i) = \|f(i)\|$.

Definition 2.7. Let $\lambda : E(\vec{G}) \rightarrow \Sigma(P)$ be a realization of G through P . A λ -orientation map is an orientation map from \vec{G} to \vec{G}' that reverses or preserves the orientation of all the edges of \vec{G} belonging to the same color class.

Given an isomorphism f from P to a pot P' , we denote by $\sigma_{f,\lambda} : E(\vec{G}) \rightarrow E(\vec{G}')$ the λ -orientation map such that $\sigma_{f,\lambda}(\vec{e}) = \vec{e}$ if and only if $f(\lambda(\vec{e})) > 0$, otherwise $\sigma_{f,\lambda}(\vec{e}) = \bar{\vec{e}}$.

The following result shows that an i -realization of a graph through a pot is preserved by isomorphic pots.

Theorem 2.8. *Let $\lambda : E(\vec{G}) \rightarrow [1, c]$ be an i -realization of G and let $P = \mathcal{P}(\lambda)$.*

- (i) *Given an isomorphism f from P to a pot P' , the map $\lambda' = f^+ \circ \lambda \circ \sigma$, with $\sigma = \sigma_{f, \lambda}^{-1}$, is an i -realization of G through P' .*
- (ii) *Given a bijection $g : \Sigma(P) \rightarrow X \subseteq \mathbb{N}$, a λ -orientation map $\sigma : E(\vec{G}) \rightarrow E(\vec{G}')$ and an automorphism ρ of G , then $\lambda' = g \circ \lambda \circ \sigma^{-1} \circ \rho$ is an i -realization of G where $\mathcal{P}(\lambda')$ is isomorphic to P and $\Sigma(\mathcal{P}(\lambda')) = X$.*

Proof. We start by proving (i). Consider the edge-coloring $\lambda' = f^+ \circ \lambda \circ \sigma$ of \vec{G}' , where $\sigma^{-1} = \sigma_{f, \lambda} : E(\vec{G}) \rightarrow E(\vec{G}')$ is the orientation map defined as follows: $\sigma_{f, \lambda}(\vec{e}) = \vec{e}$ if $f(\lambda(\vec{e})) > 0$, otherwise $\sigma_{f, \lambda}(\vec{e}) = \vec{e}$.

Since the maps f, λ and σ are all surjective, we have that $\lambda'(E(\vec{G}')) = \Sigma(P')$. We are going to show that $\tau_x(\lambda') = f(\tau_x(\lambda))$ for every $x \in V(G)$, which implies that $\mathcal{P}(\lambda') = f(P) = P'$. It is enough to notice that for every non-loop $\vec{e} \in E(\vec{G}_x)$ the following property holds: if $f(\lambda(\vec{e})) > 0$, then $\sigma^{-1}(\vec{e})_x = \vec{e}_x$ and $f^+(\lambda(\vec{e})) = f(\lambda(\vec{e}))$, otherwise $\sigma^{-1}(\vec{e})_x = -\vec{e}_x$ and $f^+(\lambda(\vec{e})) = -f(\lambda(\vec{e}))$. This implies that

$$\sigma^{-1}(\vec{e})_x \cdot f^+(\lambda(\vec{e})) = \vec{e}_x f(\lambda(\vec{e})) = f(\vec{e}_x \lambda(\vec{e})), \text{ for every } \vec{e} \in E(\vec{G}_x) \setminus L(\vec{G}_x) \quad (1)$$

and recalling that $\sigma(E(\vec{G}'_x)) = E(\vec{G}_x)$, we have that

$$\begin{aligned} \tau_x(\lambda') &= \{\vec{e}_x \cdot \lambda'(\vec{e}) \mid \vec{e} \in E(\vec{G}'_x)\} \cup \{\lambda'(\vec{e}) \mid \vec{e} \in L(\vec{G}'_x)\} \\ &= \{\vec{e}_x \cdot f^+(\lambda(\sigma(\vec{e}))) \mid \vec{e} \in E(\vec{G}'_x)\} \cup \{f^+(\lambda(\sigma(\vec{e}))) \mid \vec{e} \in L(\vec{G}'_x)\} \\ &= \{\sigma^{-1}(\vec{e})_x \cdot f^+(\lambda(\vec{e})) \mid \vec{e} \in E(\vec{G}_x)\} \cup \{f^+(\lambda(\vec{e})) \mid \vec{e} \in L(\vec{G}_x)\} \\ &\stackrel{(1)}{=} \{f(\vec{e}_x \cdot \lambda(\vec{e})) \mid \vec{e} \in E(\vec{G}_x) \setminus L(\vec{G}_x)\} \cup \{\pm f^+(\lambda(\vec{e})) \mid \vec{e} \in L(\vec{G}_x)\} \\ &= \{f(\vec{e}_x \cdot \lambda(\vec{e})) \mid \vec{e} \in E(\vec{G}_x) \setminus L(\vec{G}_x)\} \cup \{f(\lambda(\vec{e})), f(-\lambda(\vec{e})) \mid \vec{e} \in L(\vec{G}_x)\} \\ &= \{f(\vec{e}_x \cdot \lambda(\vec{e})) \mid \vec{e} \in E(\vec{G}_x)\} \cup \{f(\lambda(\vec{e})) \mid \vec{e} \in L(\vec{G}_x)\} = f(\tau_x(\lambda)), \end{aligned}$$

for every $x \in V(G)$. Therefore, λ' is a realization of G through P' .

Assuming now that λ is an i -realization of G ($i = 2, 3$), it is left to show that P' i -realizes G . For a contradiction, assume that P' realizes a graph H non-isomorphic to G whose order is either smaller than $|V(G)|$ ($i = 2, 3$) or equal to $|V(G)|$ ($i = 3$). Then, by the first part of the proof it follows that $P = \mathcal{P}(\lambda)$ realizes H (since P and P' are isomorphic), contradicting the assumption that λ is an i -realization of G .

It is left to prove (ii). Considering that $\tau_x(\lambda') = \tau_{\rho(x)}(\lambda' \circ \rho^{-1})$ for each $x \in V(G)$, it is enough to prove the assertion when ρ is the identity, that is, $\lambda' = g \circ \lambda \circ \sigma^{-1}$. It is not difficult to check that λ' is a realization of G through $P' = \mathcal{P}(\lambda')$, where $\Sigma(P') = X$. Now let $f : \Sigma(P) \cup -\Sigma(P) \rightarrow \Sigma(P') \cup -\Sigma(P')$ be the map such that $f(-i) = -f(i)$, and

$$f(i) = \begin{cases} g(i) & \text{if } \sigma \text{ fixes the orientation of all edges of the } i\text{-color class of } \lambda, \\ -g(i) & \text{otherwise,} \end{cases}$$

for each $i \in \Sigma(P)$. One can check that $f(P) = P'$, hence P and P' are isomorphic pots. By part (i), we have that P' i -realizes G , therefore λ' is an i -realization of G . \square

Remark 2.9. *We point out that Theorem 2.8.(ii) states that starting from a realization $\lambda : E(\vec{G}) \rightarrow \Sigma(P)$ of G , if we permute the colors in $\Sigma(P)$, switch the orientation of all edges of some color class of λ , or apply an automorphism of the graph G , we obtain another realization, say λ' , of G whose pot is isomorphic to P . We say that λ' is a realization of G isomorphic to λ .*

3 Known results

In this section, we recall some known facts on realizations of undirected graphs. The following result is straightforward.

Remark 3.1. *Let $\lambda : E(\vec{G}) \rightarrow [1, c]$ be a realization of an undirected graph G . We note that:*

- (i) *If G has a loop then there exists a tile $t \in \mathcal{P}(\lambda)$ such that $|-t \cap t| \geq 2$.*
- (ii) *If G has a multiple edge then there exist two tiles $t_i, t_j \in \mathcal{P}(\lambda)$ such that $|-t_i \cap t_j| \geq 2$.*

We refer the reader to Example 2.2 for an application of Remark 3.1.

Remark 3.2 [1, Section 4]. *Let $\lambda : E(\vec{G}) \rightarrow [1, c]$ be a 3-realization of an undirected loopless graph G . We note that if $\vec{e}_1, \vec{e}_2 \in E(\vec{G}_x)$ and $\lambda(\vec{e}_1) = \lambda(\vec{e}_2)$, then x is either the tail or the head of both \vec{e}_1 and \vec{e}_2 . In other words, the edges of \vec{G}_x receiving the same color from λ must be all outgoing from or all ingoing in x .*

Now we recall a very important class of graphs, the so called *Cayley graphs*. Let Γ be an additive group (not necessarily abelian) and let $\Omega \subseteq \Gamma \setminus \{0\}$ such that for every $\omega \in \Omega$, also $-\omega \in \Omega$. The Cayley graph on Γ with connection set Ω is the simple graph G defined as follows: $V(G) = \Gamma$ and $\{x, y\} \in E(G) \Leftrightarrow x - y \in \Omega$. We will denote this graph by $\text{Cay}[\Gamma : \Omega]$. It is well known that the cube graph Q can be seen as a Cayley graph on \mathbb{Z}_2^3 . To ease notation, each triple $(i, j, k) \in \mathbb{Z}_2^3$ will be denoted by ijk , and let $Q = \text{Cay}[\mathbb{Z}_2^3 : S]$, where $S = \{100, 010, 001\}$. Given an edge $\{x, y\}$ of Q and an element $g \in \mathbb{Z}_2^3$, we set $\{x, y\} + g = \{x + g, y + g\}$. Note that for every $\vec{Q} \in \text{Or}(Q)$, a tile of \vec{Q} (resp. Q) is a multiset of \mathbb{Z} of size 3.

Since the cube is a 3-regular graph, from [8] it follows that $B_1(Q) = 1$ and $T_1(Q) = 2$. Furthermore, from [1] we know that $B_2(Q) = 2$ and $T_2(Q) = 3$ and these values are simultaneously achieved by the same pot. In [1], it is also shown that a 3-realization of Q uses at least 5 colors ($B_3(Q) \geq 5$) and determines pots of size at least six ($T_3(Q) \geq 6$). The authors also construct two pots P and P' that 3-realizes Q and reach the minimum number of colors or of distinct tiles, respectively; more precisely, $|\Sigma(P)| = 5, |P| = 8$, while $|\Sigma(P')| = |P'| = 6$. Therefore, we have the following.

Lemma 3.3 [1]. $B_3(Q) = 5$ and $T_3(Q) = 6$.

In [1], the authors leave open the problem of determining whether there exists a binimal pot 3-realizing Q .

The following lemma is a restatement of [1, Lemma 4.4] in terms of color classes.

Lemma 3.4 [1, Lemma 4.4]. *Let $\lambda : E(\vec{Q}) \rightarrow [1, c]$ be a 3-realization of Q and let \mathcal{C} be the set of color classes of $\underline{\lambda}$.*

- (i) *A color class $G \in \mathcal{C}$ is either a star (with 1, 2 or 3 edges) or a matching $\{e, e + 111\}$ for some $e \in E(Q)$.*
- (ii) *\mathcal{C} contains n 3-stars (resp. 2-stars) if and only if $\mathcal{P}(\lambda)$ contains n monochromatic (resp. bichromatic) tiles.*

4 The structure of a biminimal pot that 3-realizes the cube

In this section, we provide two biminimal pots, P_1 and P_2 , that realize the cube in Scenario 3 (Propositions 4.1 and 4.2). We then show that these pots are unique up to isomorphism (Theorem 4.5).

Proposition 4.1. *The pot*

$$P_1 = \{\{1^3\}, \{2^3\}, \{-2, -3^2\}, \{-1, -4^2\}, \{-1, 3, -5\}, \{-2, 4, 5\}\}$$

is a biminimal pot that 3-realizes the cube.

Proof. Let $\lambda : E(\vec{Q}) \rightarrow [1, 5]$ be the edge-coloring of an orientation of Q inducing the pot P_1 , that is $P_1 = \mathcal{P}(\lambda)$. In Figure 3 it is shown that P_1 realizes the cube and the following table shows the tiles:

x	000	111	100	011	001, 010	101, 110
$\tau_x(\lambda)$	$\{1^3\}$	$\{2^3\}$	$\{-1, -4^2\}$	$\{-2, -3^2\}$	$\{-1, 3, -5\}$	$\{-2, 4, 5\}$

We set $t_1 = \{1^3\}$, $t_2 = \{2^3\}$, $t_3 = \{-1, -4^2\}$, $t_4 = \{-2, -3^2\}$, $t_5 = \{-1, 3, -5\}$ and $t_6 = \{-2, 4, 5\}$. First of all note that, by Remark 3.1, if G is a graph such that $G \in \mathcal{O}(P_1)$, that is, there exists $\lambda' : E(\vec{G}) \rightarrow [1, 5]$ inducing the pot P_1 , then G is a simple graph. Now we prove that G has at least 8 vertices, to do this it is useful to analyze solutions to the equations that the tiles in P_1 must satisfy. For $i = 1, \dots, 6$, denote by R_i the number of times a tile t_i appears in the realization, or, equivalently, the number of vertices in \vec{G} receiving the tile t_i , that is $R_i = |\{x \in V(G) \mid \tau_x(\lambda') = t_i\}|$. Clearly, $R_1 + \dots + R_6 = |V(G)|$. Also, as shown in [8], the R_i 's have to satisfy the following homogeneous system of linear equations:

$$\begin{aligned} 3R_1 - R_3 - R_5 &= 0 \\ 3R_2 - R_4 - R_6 &= 0 \\ -2R_3 + R_6 &= 0 \\ -2R_4 + R_5 &= 0 \\ -R_5 + R_6 &= 0 \end{aligned}$$

Therefore, $(R_1, \dots, R_6) = r(1, 1, 1, 1, 2, 2)$ and $|V(G)| = 8r$ for some integer $r \geq 1$. Hence we get $|V(G)| \geq 8$, and when $r = 1$, we have $(R_1, \dots, R_6) = (1, 1, 1, 1, 2, 2)$. So we focus on simple cubic graphs with 8 vertices and it is well known, see for instance [13], that there are exactly five graphs with

these properties. Let H be a cubic graph such that $V(H) = \{v_1, v_2, \dots, v_8\}$ and $H \in \mathcal{O}(P_1)$. Then there exists an edge-coloring $\lambda'' : E(\vec{H}) \rightarrow [1, 5]$ inducing the pot P_1 , that is

v_i	v_1	v_2	v_3	v_4	v_5, v_6	v_7, v_8
$\tau_{v_i}(\lambda'')$	$\{1^3\}$	$\{2^3\}$	$\{-1, -4^2\}$	$\{-2, -3^2\}$	$\{-1, 3, -5\}$	$\{-2, 4, 5\}$

Note that if two distinct vertices x, y are adjacent in H then there exists $j \in [1, 5]$ such that $j \in \tau_x(\lambda'')$ and $-j \in \tau_y(\lambda'')$. Hence one can directly check that $S_1 = \{v_1, v_4, v_7, v_8\}$ and $S_2 = \{v_2, v_3, v_5, v_6\}$ are two maximal disjoint independent sets of vertices of H , such that $S_1 \cup S_2 = V(H)$. In other words, the graph H is a bipartite graph with parts S_1 and S_2 . Since among the five cubic graphs of order 8 the unique bipartite graph is the cube, see [13], the graph H is the cube. \square

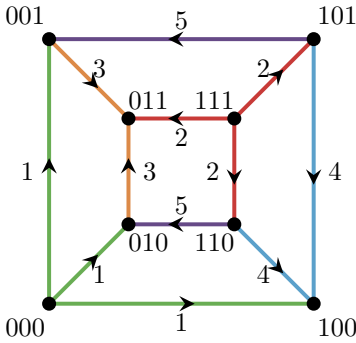


Figure 3.

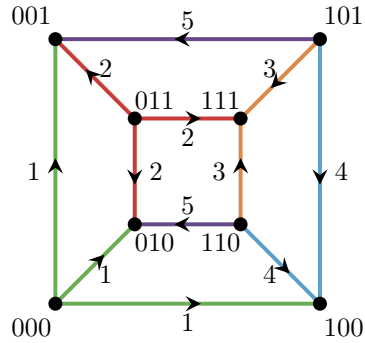


Figure 4.

Proposition 4.2. *The pot*

$$P_2 = \{\{1^3\}, \{2^3\}, \{-2, -3^2\}, \{-1, -4^2\}, \{3, 4, 5\}, \{-1, -2, -5\}\}$$

is a biminimal pot that 3-realizes the cube.

Proof. Let $\lambda : E(\vec{Q}) \rightarrow [1, 5]$ be the edge-coloring of an orientation of Q inducing the pot P_2 , that is $P_2 = \mathcal{P}(\lambda)$, see Figure 4. The following table shows the tiles:

x	000	011	111	100	101, 110	001, 010
$\tau_x(\lambda)$	$\{1^3\}$	$\{2^3\}$	$\{-2, -3^2\}$	$\{-1, -4^2\}$	$\{3, 4, 5\}$	$\{-1, -2, -5\}$

Then the result can be proved reasoning as in the proof of Proposition 4.1. \square

Remark 4.3. Note that P_1 e P_2 are non-isomorphic pots. By contradiction, assume there exists an isomorphism f between P_1 and P_2 . Recall that $f(-i) = -f(i)$ for all i in $\Sigma(P_1) \cup -\Sigma(P_1) = \Sigma(P_2) \cup -\Sigma(P_2) = \{\pm 1, \pm 2, \dots, \pm 5\}$. Then f either fixes colors 1, 2, 3, and 4, or f swaps 1 with 2 and 3 with 4. Therefore, in both cases, $f([1, 4]) = [1, 4]$. It follows that there is no tile in P_1 whose image is the tile $\{3, 4, 5\} \in P_2$.

Lemma 4.4. If P is a pot that 3-realizes Q and $|\Sigma(P)| = 5$, then P has at least two monochromatic tiles.

Proof. Let $\lambda : E(\vec{Q}) \rightarrow [1, 5]$ be a 3-realization of Q and set $P = \mathcal{P}(\lambda)$. By Lemma 3.4.(i), the color classes induced by λ on Q have size at most 3. Denoting by c_1 the number of those of size 3, we have that

$$12 = |E(Q)| = \sum_{i=1}^5 |\lambda^{-1}(i)| \leq 3c_1 + 2(5 - c_1) = c_1 + 10.$$

By Lemma 3.4.(ii), it follows that P has $c_1 \geq 2$ monochromatic tiles. \square

We now prove that the pots in Proposition 4.1 and Proposition 4.2 are the unique (up to isomorphism) biminimal pots that 3-realize the cube.

Theorem 4.5. A biminimal pot that 3-realizes the cube is necessarily isomorphic to one of the following:

- (i) $P_1 = \{\{1^3\}, \{2^3\}, \{-2, -3^2\}, \{-1, -4^2\}, \{-1, 3, -5\}, \{-2, 4, 5\}\}$;
- (ii) $P_2 = \{\{1^3\}, \{2^3\}, \{-2, -3^2\}, \{-1, -4^2\}, \{3, 4, 5\}, \{-1, -2, -5\}\}$.

Proof. Let $\lambda : E(\vec{Q}) \rightarrow [1, c]$ be a 3-realization of Q and set $P = \mathcal{P}(\lambda)$. We assume that P is biminimal, that is, $c = 5$ and $|P| = 6$. By Theorem 2.8 and Remark 2.9, it is enough to show that up to a permutation of the colors $[1, c]$, up to an automorphism of Q , and by switching (if necessary) the directions of all edges of some color classes of λ , we obtain a 3-realization of Q whose pot is either P_1 or P_2 .

Let $Q(i)$ be the i -color class determined by λ on Q , for $1 \leq i \leq 5$. By Lemma 4.4 we have that P contains at least two monochromatic tiles, say t_1 and t_2 . Up to a permutation of the colors, we may assume that $\|t_j\| = \{j^3\}$, for $j = 1, 2$. Then $Q(1)$ and $Q(2)$ contain at least three edges each; therefore, by Lemma 3.4 they are necessarily 3-stars. It is not

restrictive to assume that t_1 is the tile of vertex 000, and in view of the symmetries of the cube, we may assume without loss of generality that t_2 is the tile of either 111 or 011.

Case 1: $t_2 = \tau_{111}(\lambda)$.

Then, as shown in Figure 5, $Q \setminus \{Q_{000} \cup Q_{111}\}$ is the 6-cycle

$$C = (010, 011, 001, 101, 100, 110).$$

Note that $Q(3), Q(4), Q(5)$ can be seen as the color classes induced by $\underline{\lambda}$ on C . By Lemma 3.4, we necessarily have that each $Q(i)$, $i = 3, 4, 5$, has size exactly 2, hence each $Q(i)$ is either a 2-star or a matching $\{e, e + 111\}$ for some $e \in E(C)$. By the structure of C , if among $Q(3), Q(4), Q(5)$ there are two matchings, the third color class is a matching, as well.

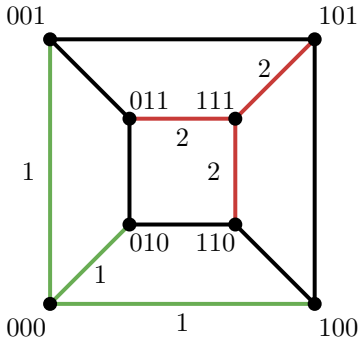


Figure 5.

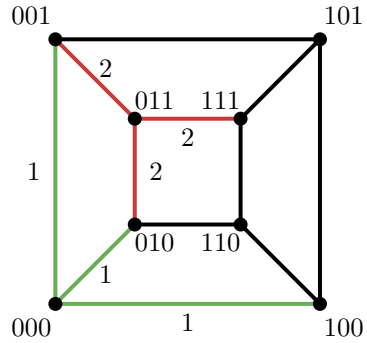


Figure 6.

Case 1.1: $Q(3), Q(4), Q(5)$ are matchings.

Up to a permutation of the colors, we may assume that

$$Q(3) = \{\{010, 011\}, \{101, 100\}\},$$

$$Q(4) = \{\{011, 001\}, \{100, 110\}\},$$

and

$$Q(5) = \{\{001, 101\}, \{110, 010\}\}.$$

The edge-coloring $\underline{\lambda}$ is then completely determined by its color classes, and one can check that $|\mathcal{P}(\underline{\lambda})| \geq 7$. By Lemma 2.3, it follows that $|\mathcal{P}(\lambda)| \geq 7$, contradicting the assumption.

Case 1.2: $Q(3), Q(4), Q(5)$ are 2-stars.

Up to a permutation of the colors and up to an automorphism of Q , we may assume that

$$\begin{aligned} Q(3) &= [010, 011, 001], \\ Q(4) &= [001, 101, 100], \\ Q(5) &= [100, 110, 010]. \end{aligned}$$

As before, one can check that $|\mathcal{P}(\lambda)| \geq 7$. By Lemma 2.3, it follows that $|\mathcal{P}(\lambda)| \geq 7$, contradicting the assumption.

Case 1.3: Among $Q(3), Q(4), Q(5)$, there are two 2-stars and one matching.

Up to a color permutation, we may assume that $Q(5)$ is the matching. Up to an automorphism of Q and a further color permutation, we may assume that

$$\begin{aligned} Q(3) &= [010, 011, 001], \\ Q(4) &= [101, 100, 110], \\ Q(5) &= \{\{001, 101\}, \{110, 010\}\}. \end{aligned}$$

One can check that

x	000	111	011	100	001, 010	101, 110
$\tau_x(\lambda)$	$\{1^3\}$	$\{2^3\}$	$\{2, 3^2\}$	$\{1, 4^2\}$	$\{1, 3, 5\}$	$\{2, 4, 5\}$

In view of Remark 3.2, by switching if necessary the directions of all edges of \vec{Q} with the same color, we can assume that the edges of \vec{Q}_{000} (resp. \vec{Q}_{111}) are all outgoing from 000 (resp. 111): hence

$$\tau_{000}(\lambda) = \{1^3\} \text{ and } \tau_{111}(\lambda) = \{2^3\}.$$

We can also assume that the two edges of \vec{Q} colored 3 (resp. 4) are ingoing in 011 (resp. 100), while the two edges colored 5 are outgoing from 101 and 110. Therefore, λ is the realization of Q shown in Figure 3, and

$$\begin{aligned} \tau_{011}(\lambda) &= \{-2, -3^2\}, \tau_{100}(\lambda) = \{-1, -4^2\}, \\ \tau_{001}(\lambda) = \tau_{010}(\lambda) &= \{-1, 3, -5\} \text{ and } \tau_{101}(\lambda) = \tau_{110}(\lambda) = \{-2, 4, 5\}. \end{aligned}$$

Case 2: $t_2 = \tau_{011}(\lambda)$.

Then, as shown in Figure 6, $Q \setminus \{Q_{000} \cup Q_{011}\}$ is the graph $G = C \cup \{e, e + 111\}$ consisting of a 4-cycle $C = (110, 111, 101, 100)$ with two pendant edges $e = \{110, 010\}$ and $e + 111 = \{001, 101\}$. Note that $Q(3), Q(4), Q(5)$ can be seen as the color classes induced by $\underline{\lambda}$ on G . By Lemma 3.4, we necessarily have that either some $Q(i)$ has size 3, or each $Q(i)$ (has size 2, hence) is either a 2-star or the matching $\{e, e + 111\}$.

Case 2.1: some $Q(i)$, $3 \leq i \leq 5$, is a 3-star.

Up to a permutation of the colors, we may assume that $Q(3)$ is a 3-star. Also, the center of $Q(3)$ is either 110 or 101. In both cases, one can check that $|\mathcal{P}(\underline{\lambda})| \geq 7$, hence (by Lemma 2.3) $|\mathcal{P}(\lambda)| \geq 7$ contradicting the assumption.

Case 2.2: $Q(3), Q(4)$ and $Q(5)$ are 2-stars.

Then, up to a permutation of the colors, we have that either

$$Q(3) = [010, 110, 111], Q(4) = [110, 100, 101], Q(5) = [111, 101, 001],$$

or

$$Q(3) = [010, 110, 100], Q(4) = [001, 101, 100], Q(5) = [110, 111, 101].$$

In both cases, one can check that $|\mathcal{P}(\underline{\lambda})| \geq 7$, hence (by Lemma 2.3) $|\mathcal{P}(\lambda)| \geq 7$ contradicting the assumption.

Case 2.3: $\{e, e + 111\}$ is a color class of $\underline{\lambda}$.

Up to a permutation of the colors, we may assume that

$$Q(5) = \{e, e + 111\}.$$

Therefore, both $Q(3)$ and $Q(4)$ are 2-stars of the 4-cycle

$$C = (110, 111, 101, 100).$$

Again, up to a color permutation, we may assume that $\{110, 111\} \in Q(3)$. If $Q(3) = [100, 110, 111]$ and $Q(4) = [111, 101, 100]$, one can check that $|\mathcal{P}(\underline{\lambda})| \geq 7$, hence (by Lemma 2.3) $|\mathcal{P}(\lambda)| \geq 7$ contradicting the assumption. Therefore, $Q(3) = [110, 111, 101]$, $Q(4) = [101, 100, 110]$, and

x	000	011	111	100	001, 010	101, 110
$\tau_x(\underline{\lambda})$	$\{1^3\}$	$\{2^3\}$	$\{2, 3^2\}$	$\{1, 4^2\}$	$\{1, 2, 5\}$	$\{3, 4, 5\}$

In view of Remark 3.2, by switching if necessary the directions of all edges of \vec{Q} with the same color, we can assume that the edges of \vec{Q}_{000} (resp. \vec{Q}_{011}) are all outgoing from 000 (resp. 011): hence

$$\tau_{000}(\lambda) = \{1^3\} \text{ and } \tau_{011}(\lambda) = \{2^3\}.$$

We can also assume that the two edges of \vec{G} colored 3 (resp. 4) are ingoing in 111 (resp. 100), while the two edges colored 5 are outgoing from 101 and 110. Therefore, λ is the realization of Q shown in Figure 4, and

$$\begin{aligned} \tau_{111}(\lambda) &= \{-2, -3^2\}, \tau_{100}(\lambda) = \{-1, -4^2\}, \\ \tau_{001}(\lambda) &= \tau_{010}(\lambda) = \{-1, -2, -5\} \text{ and } \tau_{101}(\lambda) = \tau_{110}(\lambda) = \{3, 4, 5\}. \end{aligned}$$

□

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