A METHOD FOR GENERATING COLORINGS OVER GRAPH AUTOMORPHISM

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Abstract

Given a graph \( G = (V, E) \) with a set \( W \subseteq V \) of vertices, we enumerate colorings to \( W \) such that for every two enumerated colorings \( c \) and \( c' \) the corresponding colored graphs \( (G, c) \) and \( (G, c') \) are not isomorphic. This problem has an important application in the study of isomers of chemical graphs such as generation of benzen isomers from a tree-like chemical graph structure. The number of such colorings can be computed efficiently based on Polya’s theorem. However, enumerating each from the set of these colorings without using a large space is a challenging problem in general. In this paper, we propose a method for enumerating these colorings when the automorphisms of \( G \) are determined by two axial symmetries, and show that our algorithm can be implemented to run in polynomial delay and polynomial space.

1 Introduction

Enumerating colorings of \( W \) which are not isomorphic has an important application in the study of isomers of chemical graphs such as generation of isomers of chemical graph structure. Recently Li et al. [1] designed an efficient algorithm for generating benzen isomers from a given tree-like chemical graph, where each benzen ring is contracted into a single virtual atom, to obtain an input chemical graph \( T \) with tree structure. When \( T \) has \( k \) such virtual atoms, several different chemical graphs with \( k \) benzen rings can be mapped to \( T \) by contracting the benzen rings. We call all these chemical graphs the benzen isomers of \( T \). The algorithm due to Li et al. [1] is based on dynamic programming. Their algorithm first counts the number of benzen isomers of \( T \) by a recursive structure of rooted subtrees of \( T \), and then generates each of the benzen isomers of \( T \) by a back-tracking through the counting computation. To avoid generating duplications (two isomorphic benzen isomers), all possible configurations around a benzen ring are required to be generated first. These configurations are represented by colorings of attaching carbon atoms. The idea behind Li et al.’s algorithm can be generalized to the problem of generating isomers of a tree-like chemical graph with a more complicated local structure, such as a naphthalene ring. However, generating colorings to the attaching carbon atoms of a naphthalene ring is much harder. For a benzen ring, the number of colorings is 44, whereas that for a naphthalene ring is 23,911.

In this paper, we regard the problem of generating colorings to the attaching atoms in a chemical graph as a problem of generating colorings to a subset \( W \) of vertices in a graph whose automorphisms are determined by two axial symmetries, and establish a method for generating such colorings efficiently. More formally we show that our algorithm can generate each of colorings in delay and space polynomial in \( |W| \).

The paper is organized as follows. Section 2.1 introduces basic notions on automorphisms and colorings in graphs and defines notation on symmetries and an equivalence relation among colorings. Section 2.2 proposes a method for generating colorings without duplication of equivalent colorings, and contains a proof that our algorithm can run in polynomial time and delay. Section 3 demonstrates some computation processes in the case where a given graph structure is a naphthalene ring. Section 4 makes some concluding remarks.

2 Methods

2.1 Preliminaries

2.1.1 Graphs

For two integers \( a \leq b \), let \([a, b]\) denote the set of integers \( i \) with \( a \leq i \leq b \). For a vector \( v = (e_1, e_2, \ldots, e_p) \) of nonnegative integers, the bottom index \( b(v) \) (resp., top index \( t(v) \)) is defined to be the smallest (resp., largest) index \( j \) such that \( e_j \geq 1 \). Let \( \Sigma \) be a set of symbols. Let \( G = (V, E) \) be an undirected multigraph with a vertex set \( V \) and an edge set \( E \) with no self-loops, where \( \mu(u, v) \) denotes the number of edges between two vertices \( u, v \in V \). Let \( t : V \to \Sigma \) be a type function such that \( t(v) \) of a vertex \( v \) represents the type of \( v \), i.e., an atom type in a chemical graph.

2.1.2 Symmetry

An automorphism of a graph \( G \) is a bijection \( \psi : V \to V \) such that \( t(\psi(v)) = t(v) \) for all vertices \( v \in V \) and \( \mu(\psi(u), \psi(v)) = \mu(u, v) \) holds for every pair of vertices \( u, v \in V \).

In this paper, we assume that \( G = (V, E) \) admits only two axial symmetries, \( \psi_1 \) and \( \psi_2 \), and has no other symmetries except for the identity \( \psi_0 \) or a rotational
Figure 1: Illustration for a set $W = \{w_1, w_2, \ldots, w_{24}\}$ in a graph $G$, where $\psi_1$ and $\psi_2$ are two axial symmetries that generate the four automorphisms $\psi_i$ with $i = 0, 1, 2, 3$ on $G$.

symmetry $\psi_3$ obtained by synthesizing $\psi_1$ and $\psi_2$. In other word, $G$ admits exactly four automorphisms $\psi_i$, $i = 0, 1, 2, 3$ such that:

- for $i = 0$, $\psi_0(v) = v$ for all $v \in V$;
- for $i = 1, 2$, there is a partition of $V$ into

$$X^1 = \{x_1, x_2, \ldots, x_r\}, \quad Y^1 = \{y_1, y_2, \ldots, y_s\}$$

and $Z^1 = V \setminus (X^1 \cup Y^1)$ (possibly $Z^1 = \emptyset$) such that

$$\psi_i(x_j) = y_j \quad \text{and} \quad \psi_i(y_j) = x_j, \quad j = 1, 2, \ldots, r, s,$$

and

$$\psi_i(z) = z \quad \text{for all} \quad z \in Z^1; \quad \text{and}$$

- for $i = 3$, $\psi_3 = \psi_2 \circ \psi_1$; i.e., $\psi_3(v) = \psi_2(\psi_1(v))$ for all $v \in V$.

We use the notation $\psi_i$ with $i = 0, 1, 2, 3$ in an extended way, such that for each subset $X \subseteq V$ of vertices, let $\psi_i(X)$ denote the set $\{\psi_i(v) \mid v \in X\}$.

2.1.3 Coloring Space $W$

Let $W$ be a subset of vertices in $G$ with the same vertex type, i.e., $\mathbb{E}(u) = \mathbb{E}(v)$ for every pair of vertices $u, v \in W$, such that $\psi_i(W) = \psi_2(W) = W$. We assume that there is no vertex $w \in W$ such that $\psi_i(w) = w$ for some $i \in \{1, 2, 3\}$; i.e., $W \cap Z^i = \emptyset$ for each $i = 1, 2$. Let $p = |W|$. Hence, $W$ can be partitioned into four subsets $W^{(0)}, W^{(1)}, W^{(2)}$ and $W^{(3)}$ of $p/4$ vertices, such that $W \cap X^1 = W^{(0)} \cup W^{(1)}, W \cap Y^1 = W^{(1)} \cup W^{(3)}, W \cap X^2 = W^{(0)} \cup W^{(2)}$, and $W \cap Y^2 = W^{(2)} \cup W^{(3)}$. See Fig. 1 for an illustration of $W$. Also, $W$ can be partitioned into $p/4$ subsets $Q_i$, $i = 1, 2, \ldots, p/4$ of four vertices, such that $\psi_i(Q_i) = \psi_2(Q_i) = Q_i$, where we call each $Q_i$ a block of $W$.

We label the vertices in $W$ by $w_1, w_2, \ldots, w_p$ so that $Q_i = \{w_4(i-1)+1, w_4(i-1)+2, w_4(i-1)+3, w_4(i-1)+4\}$ for all $i = 1, 2, \ldots, p/4$, and $W^{(i)} = \{w_4(i-1)+1 \mid i \in [1, p/4]\}, j = 0, 1, 2, 3$.

For example, the graph $G$ in Fig. 1 has axial symmetries $\psi_1$ and $\psi_2$ such that $\psi_1(w_1) = w_{i+1}$, $\psi_2(w_i) = w_{i+2}$, and $\psi_3(w_i) = w_{i+3}$, for each $i \in \{1, 2, \ldots, p/4\}$, and we see that the set $W = \{w_1, w_2, \ldots, w_{24}\}$ is partitioned into $W^{(0)} = \{w_1, w_5, w_9, w_{13}, w_{17}, w_{21}\}$, $W^{(1)} = \{w_2, w_6, w_{10}, w_{14}, w_{18}, w_{22}\}$, $W^{(2)} = \{w_3, w_7, w_{11}, w_{15}, w_{19}, w_{23}\}$, and $W^{(3)} = \{w_4, w_8, w_{12}, w_{16}, w_{20}, w_{24}\}$.

Fig. 3 illustrates the graph $G$ and its vertex subset $W$ for a Naphthalene ring.

2.1.4 Colorings to $W$

For a function $c : W \to [1, p]$ and an integer $i \in [1, p]$,
we denote $W_i(c) = \{w \in W \mid c(w) = i\}$, and $|c| = \max\{i \mid W_i(c) \neq \emptyset\}$. A coloring to $W$ is a function $c : W \to [1, p]$ such that

$$1 \leq |W_{c}(e)| \leq |W_{c-1}(e)| \leq \cdots \leq |W_{2}(e)| \leq |W_{1}(e)|.$$

Figure 3: Illustration for a set $W = \{w_1, w_2, \ldots, w_8\}$ in a graph $G$ of Naphthalene.
which means that \( |W_i(c)| = \emptyset \) for all \( i \in [|c| + 1, p] \).

Note that two vertices \( w, w' \in W \) adjacent in \( G \) may be assigned the same color \( c(w) = c(w') \).

See Fig. 2 for five examples of colorings \( c_i, i = 1, 2, \ldots, 5 \) to \( W \).

The color index \( \gamma(c) \) of a coloring to \( W \) is defined to be the vector \( (\gamma_1(c), \gamma_2(c), \ldots, \gamma_p(c)) \) with entries \( \gamma_j(c) = |\{ i \mid |W_i(c)| = j \}|, j = 1, 2, \ldots, p. \)

For a function \( c : W \rightarrow [1, p] \) and an automorphism \( \psi \), let \( \psi(c) \) denote the function \( c' : W \rightarrow [1, p] \) mapped from \( c \) to \( [1, p] \) by \( \psi_i \); i.e., \( c'(\psi(w)) = c(w) \) for all vertices \( w \in W \). We say that a coloring \( c \) to \( W \) is symmetric with an automorphism \( \psi \) of \( G \) if \( c = \psi[c] \); i.e., \( c(\psi_i(w)) = c'(\psi_i(w)) = c(w) \) for all vertices \( w \in W \).

We call a coloring \( c \) to \( W \) type 0 if \( c \) is not symmetric with \( \psi \) for any \( i = 1, 2, \) and type \( h \in \{1, 2, 3\} \) if \( c \) is symmetric with \( \psi \) for exactly one of \( h \) from \( \{1, 2, 3\} \); and type 4 otherwise (i.e., \( c \) is symmetric with both of \( \psi_1 \) and \( \psi_2 \)). For example, among the five colorings in Fig. 2, coloring \( c_j, j = 0, 1, 2, 3, 4 \) is of type \( j \).

For a coloring \( c \) to \( W \), if \( \gamma(c) = 1 \) for the top index of the vector \( \gamma(c) \), then a color \( i \) with \( |W_i(c)| = h \) is called the leading color. The leading coloring is always 1 by the definition of colorings. Let \( c \) be a coloring to \( W \) with leading color 1. We partition \( W_i(c) \) into a family \( W(c) \) as follows.

(I) If \( c \) is of type 0, then let \( W(c) = \{ w \mid w \in W_1(c) \} \).

(II) If \( c \) is of type \( h \) from \( h \in \{1, 2, 3\} \), then let \( W(c) = \{ w, w' \mid w, w' \in W_1(c), \psi_h(w) = w' \} \) (where \( \psi_h(w) = w' \) implies \( \psi_h(w') = w \)).

(III) If \( c \) is of type 4, then let \( W(c) = \{ u_1, u_2, u_3, u_4 \mid u_1, u_2, u_3, u_4 \in W_1(c), \psi_1(w) = u_2, \psi_1(w) = u_4, \psi_2(u_1) = u_3 \} \) (where \( \psi_1(u_1) = u_2, \psi_1(u_3) = u_4 \) and \( \psi_2(u_1) = u_3 \) imply \( \psi_2(u_2) = u_4 \), and each subset \( P \in W(c) \) is a block of \( W \).

In (III), we denote each subset \( P \in W(c) \) by an ordered set \( (u_1, u_2, u_3, u_4) \) such that \( \psi(u_1) = u_2, \psi_2(u_1) = u_3 \) and \( \psi_3(u_1) = u_4 \); i.e., \( \{ u_j \} \in P \cap W^{(j)} \), \( j = 1, 2, 3, 4 \).

For the five colorings in Fig. 2, each of which has the leading color 1, we have

\( W(c_0) = \{ w_1, \{ w_2, \{ w_3, \{ w_4, \{ w_5, \{ w_6, \{ w_7, \{ w_8, \{ w_9 \} \} \} \} \} \} \} \} \),

\( W(c_1) = \{ w_1, \{ w_2, \{ w_3, \{ w_4, \{ w_5, \{ w_6, \{ w_7, \{ w_8, \{ w_9 \} \} \} \} \} \} \} \} \),

\( W(c_2) = \{ w_1, \{ w_2, \{ w_3, \{ w_4, \{ w_5, \{ w_6, \{ w_7, \{ w_8, \{ w_9 \} \} \} \} \} \} \} \} \),

\( W(c_3) = \{ w_1, \{ w_2, \{ w_3, \{ w_4, \{ w_5, \{ w_6, \{ w_7, \{ w_8, \{ w_9 \} \} \} \} \} \} \} \} \),

\( W(c_4) = \{ w_1, \{ w_2, \{ w_3, \{ w_4, \{ w_5, \{ w_6, \{ w_7, \{ w_8, \{ w_9 \} \} \} \} \} \} \} \} \),

\( \{ w_{10}, w_{11}, w_{12}, w_{13}, w_{14}, w_{15}, w_{16}, w_{17}, w_{18}, w_{19}, w_{20} \} \).

2.1.5 Equivalence of Colorings

We say that two colorings \( c \) and \( c' \) are equivalent if there is an automorphism \( \gamma \) of \( G \) such that \( c(w) = c'(\psi(w)) \) for all vertices \( w \in W \). We denote by \( c \equiv c' \) that \( c \) and \( c' \) are equivalent. Obviously two colorings \( c \) and \( c' \) to \( W \) cannot be equivalent if \( \gamma(c) = \gamma(c') \) or \( c \) and \( c' \) are of different types. However, the converse is not true in general.

A vector \( k = (k_1, k_2, \ldots, k_p) \) with \( p \) entries of nonnegative integers is called an index vector if \( \sum_{i=1}^p k_i = p \). Let \( I_p \) denote the set of all index vectors with \( p \) entries. For an index vector \( k \in I_p \), let \( C(k) \) denote the set of all colorings \( c \) such that \( \gamma(c) = k \).

Note that the relation \( \equiv \) partitions the set \( C(k) \) into equivalence classes \( C_1(k), C_2(k), \ldots, C_{\kappa(k)}(k) \), where \( \kappa(k) \) denotes the number of classes in \( C(k) \).

Our goal is to generate exactly one coloring from each equivalence class \( C_j(k), j \in I_p \). For this, we define a “canonical coloring” to be a representative from each equivalence class \( C_j(k) \).

For each subset \( S \subseteq W \), let \( s(S) \) be the sequence \( (i_1, i_2, \ldots, i_{|S|}) \) of labels of vertices in \( S = \{ w_1, w_2, \ldots, w_{|S|} \} \) such that \( i_j < i_r \) holds for \( 1 \leq j < r \leq |S| \).

A label sequence \( s(c) \) of a coloring \( c \) to \( W \) is defined to be the concatenation

\( (s(W_1(c)), s(W_2(c)), \ldots, s(W_{|c|}(c))) \)

of sequences \( s(W_i(c)) \), \( i = 1, 2, \ldots, |c| \). A coloring \( c \) is called canonical if \( s(c) \) is lexicographically smaller than \( s(c') \) for any other coloring \( c' \) equivalent to \( c \).

Let \( C^*(k) \) be the set of all canonical colorings \( c \subseteq C(k) \) for an index vector \( k \in I_p \).

2.2 Generating Canonical Colorings

We generate canonical colorings to \( W \) systematically, so that a coloring \( c \) is obtained from a coloring \( c' \) with \( |c'| = |c| - 1 \). For this, we use the idea of family trees [2, 3], based on which we introduce a parent-child relationship \( \pi \) among objects to be enumerated. We span all the objects with a tree \( T \) rooted at a designated object in such a way that each of the other objects is a descendant of \( T \) in the parent-child relationship \( \pi \).

2.2.1 Parent of Colorings

To introduce a parent-child relationship among colorings to \( W \), we define the parent of a coloring \( c \) such that \( \gamma(c) = 0 \). Change the color of each vertex in \( W_{|c|}(c) \) into 1 to obtain a new coloring \( c' \) with \( |c'| = |c| - 1 \); i.e.,

\[
\gamma'(w) = \begin{cases} 
1 & \text{for all } w \in W_{|c|}(c) \\
\gamma(w) & \text{for all } w \in W \setminus W_{|c|}(c).
\end{cases}
\]

Define the parent \( \pi(c) \) of \( c \) to be the coloring \( c' \), and call \( c \) a child of \( c' \). Let \( Ch(c') \) be the set of all children of \( c' \), and \( c_{\text{root}} \) be the coloring such that \( \gamma_p(c_{\text{root}}) = 1 \).
Figure 4: The family tree of all 21 index vectors in $I_8$.

Note that every coloring $c' = \pi(c)$ that is the parent of some coloring $c$ has a leading color since $\gamma_2(c') = 1$ for the top index $t(k)$ of $k = \gamma(c')$. We design a method that generates all children of a given coloring $c$.

2.2.2 Parent of Index Vectors

To facilitate generating all children of a given coloring $c$, we also introduce a parent-child relationship among index vectors. Define $k_{\text{root}}$ to be the index vector $(0, 0, \ldots, 1) \in I_p$, and the parent $\pi(k)$ of an index vector $k \in I_p \setminus \{k_{\text{root}}\}$ as follows. Let $b = b(k)$ and $t = t(k)$ be the bottom and top indices of $k$. Then the parent $\pi(k)$ of $k$ is defined to be the index vector $k' \in I_p$ such that:

- $k'_b = k_b - 1$ and $k'_t = k_t - 1$ for $b' = t$,
- $k'_{b+1} = k_{b+1} + 1$ (i.e., 1), and
- $k'_i = k_i$ for $i \in [1, p] \setminus \{b, t, b + t\}$.

A vector $k'' \in I_p$ is called a child of a vector $k' \in I_p$ if $k' = \pi(k'')$, and let $\mathcal{Ch}(k')$ be the set of all children of $k'$. Note that, for any vector $k \in I_p$, it holds $\mathcal{Ch}(k') = \emptyset$ if $k_t(k) = 1$.

The family tree of $I_8$ given by the above definition is given in Fig. 4.

For two colorings $c$ and $c' = \pi(c)$, we see that their color indices $k = \gamma(c)$ and $k' = \gamma(c')$ satisfy $k' = \pi(k)$, by the definition of parents of colorings and index vectors. From this observation, when we generate colorings in $\mathcal{Ch}(c)$ of a coloring $c$, we first generate index vectors $k \in \mathcal{Ch}(c)$ of the color index $k = \gamma(c)$, and then construct colorings $\hat{c}$ with $\gamma(\hat{c}) = k$.

2.2.3 Generating Colorings with the Root Index Vectors

We here show how to generate colorings in $C^*(k_{\text{root}})$ for the root $k_{\text{root}}$. Note that the $p$-th entry of $k_{\text{root}}$ is 1. Hence $C^*(k_{\text{root}})$ consists of a single coloring $c_{\text{root}}$ such that $c(w) = 1$ for all vertices $w$ in $W$, and it holds $\{c_{\text{root}}\} = C^*(k_{\text{root}})$. Fig. 5 illustrates the coloring $c \in C^*(k_{\text{root}})$ with $k_{\text{root}} = (0, 0, 0, 0, 0, 0, 0, 0, 1)$ in the graph in Fig. 3.

2.2.4 Generating Colorings with Non-root Index Vectors

We now show how to generate canonical colorings in $\mathcal{Ch}(c)$ for a given canonical coloring $c$ with leading color $1$. Recall that a coloring $c$ with leading color 1 admits the family $W(c) = \{P_1, P_2, \ldots, P_m\}$, which is a partition of $W_1(c)$. Let $k' = \gamma(c)$ and $t = |W_1(c)|$ be the top index $t(k')$ of $k'$. We fix a child $k \in \mathcal{Ch}(k')$ to generate colorings $\hat{c} \in \mathcal{Ch}(c)$ such that $\gamma(\hat{c}) = k$. Let $b = b(k)$ and $t = t(k)$ be the bottom and top indices of $k$, where $b \leq t$ and $t = b + t$. This means that a child $\hat{c} \in C(k)$ of $c$ can be obtained by changing the colors of some $b$ vertices in the subset $W_1(c)$ into a new color $|c| + 1$.

We show how to choose $b$ vertices from $W_1(c)$ to avoid generating two equivalent colorings in $C(k)$.

Let $\beta(c, b)$ be the set of all vectors $b = (b_1, b_2, \ldots, b_m)$ such that $b_i \in [0, |P_i|]$ for each $P_i \in W(c) = \{P_1, P_2, \ldots, P_m\}$ and $\sum_{i \leq m} b_i = b$.

A vector $(b_1, b_2, \ldots, b_m) \in \beta(c, b)$ means that we choose exactly $b_i$ vertices from $P_i$ for each $i = 1, 2, \ldots, m$. For both $\beta(c, b)$, let $Z(c, b)$ denote the family of subsets $Z \subseteq W_1(c)$ such that $Z \cap P_i = b_i$ for all $i = 1, 2, \ldots, m$. For a set $Z \in Z(c, b)$, let $c/Z$ denote the coloring $\hat{c}$ to $W$ such that

$$
\hat{c}(w) = \begin{cases} |c| + 1 & \text{for all } w \in Z \\ c(w) & \text{for all } w \in W \setminus Z \end{cases}
$$

The maximum possible number of choices of $b_i$ vertices from $P_i$ for each $i$ is $|P_i|$, and the maximum possible number of colorings $\hat{c} \in C(k)$ constructed in this way is $|\Pi_{i \in [1, m]} (|P_i| + 1)|$, which is $|Z(c, b)|$. Note that some $Z, Z' \in Z(c, b)$ may produce two colorings $c/Z$ and $c/Z'$ which are equivalent. So we need to avoid such duplications.

A subfamily $Z' \subseteq Z(c, b)$ is called proper if

(i) for every two sets $Z, Z' \in Z'$, colorings $c/Z$ and $c/Z'$ are not equivalent; and

(ii) for any set $Z \in Z(c, b) \setminus Z'$, there is a set $Z' \in Z'$ such that any coloring $c/Z$ is equivalent to the corresponding coloring $c/Z'$.

To construct a proper subfamily $Z' \subseteq Z(c, b)$, we distinguish three cases according to the type of the coloring $c$.

Case (I): $c$ is of type 0. Now $W(c) = \{P_1, P_2, \ldots, P_m\} = \{w\}$ if $w \in W_1(c)$. In this case, $0 \leq b_i \leq 0$.
1 = |P_i| for all i = 1, 2, ..., m, and Z(c, b) = \{Z\} holds for the set Z of vertices chosen from W_1(c); i.e., Z = u_i \cup b_1=1 P_i, where c = c/Z is also of type 0. In this case, let Z' = \{Z\}.

Case (II): c is of type h \in \{1, 2, 3\}: Now W(c) = \{P_1, P_2, ..., P_m\} = \{w, w'\} \cup w, w' \in W_1(c), \psi(w) = w'\}. In this case, 0 \leq b_i \leq 1 = |P_i| for all i = 1, 2, ..., m. We distinguish two subcases.

(II-a) b_j \in \{0, 2\} for all i \in \{1, 2, ..., m\}. In this case, Z(c, b) = \{Z\} holds for the set Z = U_i \cup b_{i=2} P_i of vertices chosen from \{W_1(c)\}, where c = c/Z is also of type h. In this case, let Z' = \{Z\}.

(II-b) b_j = 1 for some j \in \{1, 2, ..., m\}: We fix such an index j and a vertex v_j from P_j arbitrarily. Let S be the family of sets S \subseteq W_1(c)P_j such that [S \cap P_i] = b_i for all i \in \{1, 2, ..., m\} \setminus \{j\}, where [S] = \Pi_i \cap b_i \neq 1, i

\{S_i \subseteq S \subseteq S\}, where c = c/Z is of type 0 for any Z' \in Z'.

Case (III): c is of type 4: Now W(c) = \{u_1, u_2, u_3, u_4\} \cup u_1, u_2, u_3, u_4 \in W_1(c), \psi(u_1) = u_2, \psi(u_3) = u_2, \psi(u_4) = u_4, \psi(u_1) = u_3\}.

We distinguish three subcases.

(III-a) b_j \in \{1, 3\} for some j \in \{1, 2, ..., m\}: We fix such an index j and a subset F_j \subseteq P_j of b_j vertices arbitrarily. Let S be the family of sets S \subseteq W_1(c)P_j such that [S \cap P_i] = b_i for all i \in \{1, 2, ..., m\} \setminus \{j\}, where [S] = \Pi_i \cap b_i \neq 1, i

\{S_i \subseteq S \subseteq S\}. For each \{S_i \subseteq S \subseteq S\}, where \psi = \psi/Z is also of type 4. In this case, let Z' = \{Z\}.

(III-b) b_j \in \{0, 4\} for all i \in \{1, 2, ..., m\}. In this case, Z(c, b) = \{Z\} holds for the set Z of vertices chosen from \{W_1(c)\}; i.e., Z = U_i \cup b_{i=4} P_i, where c = c/Z will be of type h = 0, 1, or 2.

(1) Let b \in \{1, 2, 3\}. We fix an index j with b_j = 2. For each i \in \{1, 2, ..., m\} such that b_i = 2, we fix a set F_i of two vertices u, v \in P_i such that \psi(u) = u', \psi(v) = v. Let S_b be the family of sets S \subseteq \{W_1(c)\} such that [S \cap P_i] = b_i for all i \in \{1, 2, ..., m\} \setminus \{j\}, and [S \cap F_i] \in \{0, 2\} for each i \in \{1, 2, ..., m\} \setminus \{j\} with b_i = 2, where [S_b] = \Pi_i \cap b_i \neq 2, i

\{S_i \subseteq S \subseteq S\}\}. In this case, let Z'_b = \{P_i \cup b \cup S \subseteq S_b\}.

(2) Consider the case of h = 0, which means that there are two indices j and r such that b_j = b_r = 2 (Z_0 is set to be \emptyset if no two indices exist). Without loss of generality assume that b_1 = 2 for i \in \{1, m\}' and b_i \in \{0, 4\} for i \in \{m'+1, m\}. For each P_i = \{u_1, u_2, u_3, u_4\} with i \in \{1, m\}', define

P_i^{(1)} = \{u_1, u_2\}, P_i^{(2)} = \{u_1, u_3\}, P_i^{(3)} = \{u_1, u_4\}, and

P_i^{(r)} = P_i \backslash P_i^{(r)} r, 1, 2, 3,

where \psi_i(P_i^{(r)}) = P_i^{(r)} and \psi_i(P_i^{(r)}) = P_i^{(r)} for each r = 1, 2, 3.

For each set Z \in Z_0(c, b), coloring c of type 4 becomes a coloring c/Z of type 0, and there is a tuple (j, r, q) of an index j \in \{2, m\}' and integers r, q \in \{1, 3\} with \psi = \psi such that

\begin{align*}
Z \cap P_i \in \{U_i^{(r)} P_i^{(r)}\} \quad & \text{for all } i \in \{1, j - 1\} \\
\text{and} \\
Z \cap P_j \in \{P_j^{(q)} P_j^{(q)}\}.
\end{align*}

We call such an index j the pivot of Z.

For each r \in \{1, 2, 3\} and j \in \{2, m\}', define

A_{j, r} = \{u_2 \leq s \leq l S_i \in P_i^{(r)} P_i^{(r)}\},

where A_{j, r} = \emptyset and |A_{j, r}| = 2^{j - 2}. For each j \in \{2, m\}', define

B_{j} = \{u_j \leq s \leq l S_i \in P_i, |S_i \cap P_i| = 2\},

where B_{m'} = \emptyset and |B_{j}| = 6^{m' - r}. Denote

\begin{align*}
C = \bigcup_{i \in \{m' + 1, m\}, i \neq 1} P_i.
\end{align*}

Define

\begin{align*}
R_0 = \{(1, 2), (2, 1), (1, 3), (3, 1), (2, 3), (3, 2)\}, \\
R_1 = \{(1, -2), (-2, 1), (1, -3), (-3, 1), (-2, -3), (-3, -2)\}, \\
R_2 = \{(-1, 2), (2, -1), (-1, -3), (-3, -1), (2, -3), (-3, -2)\},
\end{align*}

and

\begin{align*}
R_3 = \{(-1, -2), (-2, -1), (-1, -3), (-3, -1), (-2, 3), (3, -2)\}.
\end{align*}

For each j \in \{2, m\}' and (s, t) \in R_0 \cup R_1 \cup R_2 \cup R_3, define

P_{j, (s, t)} = \{P_j^{(s)} \cup A \cup P_j^{(r)} \cup B \cup C \mid C \subseteq A \cup A_j, j \neq 1, B \subseteq B_j\}.

Define

\begin{align*}
Z_i = \bigcup_{j \in \{2, m\}', (s, t) \in R_i} P_{j, (s, t)}, \quad i = 0, 1, 2, 3.
\end{align*}

Then we see that

\begin{align*}
Z_0(c, b) = \bigcup_{i=0, 1, 2, 3} Z_i.
\end{align*}

We define a subfamily Z'_b to be Z'_0(2).

From the constructions in (1) and (2), let Z' = U_{b_1=0,1,2,3} Z'_b.

This completes our method of constructing a subfamily Z' of Z(c, b). We show that the above subfamily Z' is proper.

Theorem 1 The family Z' defined above is a proper subfamily of Z(c, b).
Proof. Since two colorings of different types cannot be equivalent, a subfamily $Z'$ of $Z(c, b)$ is proper if the above conditions hold for each type of colorings $c/Z$ with $Z \in Z(c, b)$. More formally, for each $h = 0, 1, 2, 3$, let

$$Z_h(c, b) = \{ Z \in Z(c, b) \mid c/Z \text{ is of type } h \}.$$ 

Then a subfamily $Z'$ of $Z(c, b)$ is proper if and only if for each $h = 0, 1, 2, 3$

(1-h) for every two sets $Z, Z' \in Z' \cap Z(h,c, b)$, colorings $c/Z$ and $c/Z'$ are not equivalent; and

(2-h) for any set $Z \in Z_h(c, b) \setminus Z'$, there is a set $Z'' \in Z' \cap Z_h(c, b)$ such that the coloring $c/Z$ is equivalent to the coloring $c/Z''$, where $c/Z$ and $c/Z'$ are of type $h$.

For cases (I), (II-a) and (III-b), where $Z' = Z(c, b)$ contains a single set, the theorem holds.

We distinguish cases (II-b), (III-a) and (III-c).

Case (II-b). $c$ is of type $h \in \{1, 2, 3\}$. We have fixed an index $j$ with $b_j = 1$ and a vertex $P_j \in P$, where we denote $P_j = \{s_j, \bar{s}_j\}$. Since $c$ is symmetric with $\psi_h$, and $|Z \cap P_j| = 1$ holds for all sets $Z \in Z(c, b)$, we see that every coloring $c/Z$ with $Z \in Z(c, b)$ is of type 0; i.e., $Z(c, b) = Z_0(c, b)$. Let $S_2 = U_{i=1, b_i=1} P_i$ and $S_1$ be the family of sets $S \subseteq U_{i=1, b_i=1, i \neq j} P_i$ such that $|S \cap P_i| = 1$ for all $i(= j)$ with $b_i = 1$ and $|S| = \Pi_{b_i=1, i \neq j} 2$. Hold note that for every set $S \in S_1$, the set $U_{i=1, b_i=1, i \neq j} P_i \setminus S$ belongs to $S_1$. Then the family $Z'$ is given by $Z' = \{ s_j \} \cup S_2 \cup S \cup S_2 \cup S_1$. Define

$$Z'' = \{ s_j \} \cup S_2 \cup S \cup S_1.$$ 

Then $Z(c, b)$ is given by $Z'' \cup Z''$. For each set $S = \{ s_j \} \cup S_2 \cup S$, where $S \in S_1$, define the set

$$Z = \{ s_j \} \cup S_2 \cup U_{(i: b_i=1, i \neq j)} P_i \setminus S,$$ 

which belongs to $Z''$, and we see that $\psi_h[c/Z] = c/Z$ since $c$ is symmetric with $\psi_h$. This means that $\{ c/Z \mid Z \in Z(c, b) \}$ is partitioned into two sets $C_0 = \{ c/Z \mid Z \in Z'' \}$ and $C_1 = \{ c/Z \mid Z \in Z'' \}$ such that every coloring in $C_0$ is equivalent to a coloring in $C_1$. Therefore, every set $Z \in Z(c, b) \setminus Z'$ admits a set $Z'' \in Z'' \cup Z''$ such that every coloring in $C_0$ is equivalent to a coloring in $C_1$. Therefore, every set $Z \in Z(c, b) \setminus Z'$ admits a set $Z'' \in Z'' \cup Z''$ such that every coloring in $C_0$ is equivalent to a coloring in $C_1$. Since $c$ is of type $h \in \{1, 2, 3\}$ and thereby each coloring $c/Z$ with $Z \in Z(c, b)$ is equivalent to at most one coloring $c/Z'$ with $Z \in Z(c, b)$, this means that, for every two sets $Z, Z'' \in Z'' \cup Z''$, colorings $c/Z$ and $c/Z'$ are not equivalent. Hence $Z'$ is a proper subfamily of $Z(c, b)$.

Case (III-a) $c$ is of type 4 and there exists an index $j$ such that $b_j \in \{1, 3\}$. For such an index $j$, block $P_j$ is no longer automorphic in $c/Z$ for any set $Z \in P_j \in \{1, 3\}$, implying that $Z(c, b) = Z_0(c, b)$. We have fixed an index $j$ with $b_j \in \{1, 3\}$ and a subset $F_j \subseteq P_j$ of $b_j$ vertices. Note that the three other choices of $b_j$ vertices from $P_j$ are given by $\psi_1(F_j), \psi_2(F_j)$ and $\psi_3(F_j)$. Hence, $Z(c, b)$ and our choice of a subfamily $Z'$ are given as follows. Let $S_2 = U_{i: b_i=4} P_i$ and $S_1$ be the family of sets $S \subseteq U_{i: b_i=1, i \neq j} P_i$ such that $|S \cap P_i| = b_i$ for all $i(= j)$ where $|S_1| = \Pi_{b_i=1, i \neq j} 4$ · ($b_{j=1}$) holds, and for each set $S \in S_1$ and $h \in \{1, 2, 3\}$, it holds $\psi_h(S) \in S_1$. Define

$$Z(h) = \{ \psi_h(F_j) \cup S_2 \cup S \mid S \in S_1 \} \text{ for } h = 0, 1, 2, 3.$$

Then $Z(c, b)$ is given by $U_{h=0, 1, 2, 3} Z(h)$, and the family $Z'$ is given by $Z(0)$.

For each set $Z = F_j \cup S_2 \cup S$ with $S \in S_1$ and $h \in \{1, 2, 3\}$, define the set

$$Z(h) = \psi_h(F_j) \cup S_2 \cup \psi_h(S),$$

which belongs to $Z(h)$, and we see that $\psi_h[c/Z] = c/Z(h)$, since $c$ is symmetric with $\psi_h$. This means that $\{ c/Z \mid Z \in Z(c, b) \}$ is partitioned into four sets $C_h = \{ c/Z \mid Z \in Z(h) \}$, $h = 0, 1, 2, 3$ such that every coloring in $C_0$ is equivalent to a coloring in each of $C_1, C_2$ and $C_3$. Therefore, for each $h \in \{1, 2, 3\}$, every set $Z \in Z(h) \subseteq Z(c, b) \setminus Z'$ admits a set $Z'' \in Z'' \cup Z''$ such that the coloring $c/Z$ is equivalent to the coloring $c/Z''$. Since $c$ is of type 4 and thereby each coloring $c/Z$ with $Z \in Z(c, b)$ is equivalent to at most three colorings $c/Z_1, c/Z_2$ and $c/Z_3$ with $Z_1, Z_2, Z_3 \in Z(c, b) \setminus Z'$. This means that, for every two sets $Z, Z'' \in Z'' \cup Z''$, colorings $c/Z$ and $c/Z'$ are not equivalent. Hence $Z'$ is a proper subfamily of $Z(c, b)$.

Case (III-c) $c$ is of type 4 and $b_i \in \{0, 2, 4\}$ for all $i \in \{1, 2, \ldots, m\}$; For each $h = 0, 1, 2, 3$, we see that $Z_h \subseteq Z_h(c, b)$, and it suffices to show that $Z_h$ satisfies the conditions (1-h) and (2-h).

(1) Let $h \in \{1, 2, 3\}$. We have fixed an index $j$ with $b_j = 2$ and a set $F_j = \{ u, u' \} \subseteq P_j$ such that $\psi_h(u) = u'$ for each $i \in \{1, 2, \ldots, m\}$ with $b_i = 2$. The family $Z_h(c, b)$ and our choice of subfamily $Z_h$ are given as follows. Let $S_4 = U_{i: b_i=2} P_i$, and $S_1$ be the family of sets $S \subseteq U_{i: b_i=2, i \neq j} P_i$ such that $|S \cap P_i| = 2$ for all $i \in \{1, 2, \ldots, m\}$ with $b_i = 2$. Note that for every set $S \in S_2$, the set $(U_{i: b_i=2, i \neq j} P_i) \setminus S$ belongs to $S_2$. Let

$$Z_h' = \{ (P_j \setminus F_j) \cup S_2 \cup S \mid S \in S_2 \}.$$ 

Then the family $Z_h(c, b)$ is given by $Z_h' \cup Z_h'$. For each set $Z = F_j \cup S_2 \cup S$ with $S \in S_2$, define the set

$$Z = \{ P_j \setminus F_j \cup S_2 \cup (U_{i: b_i=2, i \neq j} P_i) \setminus S \},$$

which belongs to $Z_h(c, b)$, where we see that $\psi_i[c/Z] = c/Z$ for $i \in \{1, 2, 3\} \setminus \{h\}$. This means that $Z_h(c, b)$ is partitioned into two sets $C_0 = \{ c/Z \mid Z \in Z_h' \}$ and $C_1 = \{ c/Z \mid Z \in Z_h' \}$ such that every coloring in $C_0$ is equivalent to a coloring in $C_1$ in that they are symmetric with $\psi_h$. Therefore condition (2-h) holds.
Since every coloring $c/Z$ with $Z \in Z_h(c, b)$ is of type $h$, each coloring $c/Z$ with $Z \in Z_{h}'$ is equivalent to at most one coloring $c/Z'$ with $Z' \in Z'_{h}$. This means that condition (1-h) holds.

(2) $h = 0$: When some sets $Z, Z' \in Z_{0}(c, b)$ produce equivalent colorings $c/Z$ and $c/Z'$, their pivots must be the same. Hence, fix an index $j \in [2, m']$, and consider the equivalence among colorings $c/Z$ only for sets $Z \in Z_0(c, b)$ with pivot $j$.

For a set $S = P_i^{(s)} \subseteq P_i$, with $i \in [1, m']$ and $s \in \{-3, -2, -1, 1, 2, 3\}$ and $\ell \in [1, 3]$, we define

$$S^{(\ell)} = \begin{cases} P_i^{(s)} & \text{if } |s| = \ell \\ P_i^{(-s)} & \text{otherwise} \end{cases}$$

where it holds $\psi_i(P_i^{(s)}) = S^{(\ell)}$. For a set $X = U_{x \in J} S_x$ that consists of $S_x = P_x^{(s)}$, where $s_x \in \{-3, -2, -1, 1, 2, 3\}$ for some index set $J \subseteq [1, m']$, we denote by $X^{(\ell)}$ the union $U_{x \in J} S_x^{(\ell)}$.

For each set $B \in b_j$, and an integer $\ell \in [1, 3]$, we see that the set $B^{(\ell)}$ satisfies $\psi_i(B) = B^{(\ell)}$ and belongs to $b_j$. Analogously, for each set $A \in a_i$, with $r \in [1, 2, 3]$, the set $A^{(r)}$ satisfies $\psi_r(A) = A^{(r)}$ and belongs to $A_{i,j,r}$.

Let $X = P_i^{(s)} \cup P_j^{(t)}$ be a set such that $s, t \in \{-3, -2, -1, 1, 2, 3\}$, $s ≠ t$ and $1 \leq x < y \leq m'$. Then we observe the following:

- If $(s, t) \in R_0$ (resp., $R_2$), then $X$ is mapped to $\psi_1(X) = X^{(1)}$, and $X^{(1)}$ belongs to $R_1$ (resp., $R_3$);
- If $(s, t) \in R_0$ (resp., $R_2$), then $X$ is mapped to $\psi_2(X) = X^{(2)}$, and $X^{(2)}$ belongs to $R_2$ (resp., $R_3$); and
- If $(s, t) \in R_0$ (resp., $R_1$), then $X$ is mapped to $\psi_3(X) = X^{(3)}$, and $X^{(3)}$ belongs to $R_3$ (resp., $R_2$).

This means that:

- each set $Z \in Z^{(0)}$ (resp., $Z^{(2)}$) is mapped to $\psi_1(Z) \in Z^{(1)}$ (resp., $Z^{(3)}$);
- each set $Z \in Z^{(0)}$ (resp., $Z^{(1)}$) is mapped to $\psi_2(Z) \in Z^{(2)}$ (resp., $Z^{(3)}$); and
- each set $Z \in Z^{(0)}$ (resp., $Z^{(1)}$) is mapped to $\psi_3(Z) \in Z^{(2)}$ (resp., $Z^{(3)}$).

Recall that the above argument holds for any fixed pivot $j \in [2, m']$. This means that conditions (1-0) and (2-0) hold for $Z_j^{(0)} = Z^{(0)}$.

Based on Theorem 1, we obtain the next theorem.

**Theorem 2** For a canonical coloring $c$, an index vector $k \in Ch(\gamma(c))$ and a vector $b \in \beta(c, b(k))$, let $Z_{c,b}^{(0)}$ be a subfamily of $Z_{c,b}$. Then it holds that $Ch(c) = U_{k \in Ch(\gamma(c))} U_{b \in \beta(c, b(k))} \{c/Z \mid Z \subseteq Z_{c,b}^{(0)}\}$.

**Proof.** First we prove that, given a canonical coloring $c$, an index vector $k \in Ch(\gamma(c))$, and two distinct vectors $b = (b_1, b_2, \ldots, b_m), b' = (b'_1, b'_2, \ldots, b'_m) \in \beta(c, b(k))$, a coloring $c/Z$ with $Z \in Z_{c,b}$ is not equivalent to any coloring $c/Z'$ with $Z' \in Z_{c,b'}$. Since $b \neq b'$, there must exist some integer $i \in \{1, 2, \ldots, m\}$ such that $b_i \neq b'_i$. For the set $P_i \in W(c)$, it holds $[Z \cap P_i] = b_i' = b'_i = [Z' \cap P_i]$. This means that the colorings $c/Z$ and $c/Z'$ are not equivalent even over the block $Q = P_i$.

Next we prove that no two colorings $\hat{c}_1, \hat{c}_2 \in Ch(c)$ with $\gamma(\hat{c}_1) = \gamma(\hat{c}_2)$ are equivalent. From the parent-child relationship of index vectors, we can see that for any two $k, k' \in Ch(\gamma(c))$ with $k \neq k'$, it holds that $b(k') = b(k')$. Then for any two vectors $b = (b_1, b_2, \ldots, b_m) \in \beta(c, b(k))$ and $b' = (b'_1, b'_2, \ldots, b'_m) \in \beta(c, b(k'))$, it holds that $\sum_{i=1}^{m} b_i = b(k') = b(k') = \sum_{i=1}^{m} b'_i$. Therefore $b = b'$, and we see that $\hat{c}_1$ and $\hat{c}_2$ are not equivalent, as observed above.

Therefore, given a canonical coloring $c$, no two colorings $\hat{c}_1, \hat{c}_2 \in Ch(c)$ are equivalent and it always holds that $\pi(\hat{c}) = c$ where $\hat{c} = c/Z$ with $Z \in Z_{c,b}^{(0)}$ and $b \in \beta(c, b(k))$ with $k = \gamma(c)$. Hence, it holds that $Ch(c) = U_{k \in Ch(\gamma(c))} U_{b \in \beta(c, b(k))} \{c/Z \mid Z \subseteq Z_{c,b}^{(0)}\}$. □

**PROCEDURE**
Input: A canonical coloring $c$ with a leading color.
Output: All canonical colorings in $Ch(c)$.
Let $k' := \gamma(c)$;
for each child $k \in Ch(k')$
do
Let $b = b(k)$ be the bottom index of $k$;
for each $b \in \beta(c, b)$
/* Let $Z'$ be a proper subfamily of $Z(c, b)$ */
for each set $Z \in Z'_{c,b}$
do
$\hat{c} := c/Z$;
Output the canonical coloring $\hat{c}$
of the set of colorings equivalent to $\hat{c}$
end for
end for

2.2.5 Algorithm
Based on the procedure for generating all canonical colorings that are children of a canonical coloring, we can obtain an algorithm for enumerating all canonical colorings to $W$. By applying the following recursive procedure $\text{GENERATE}(c)$ to the canonical coloring $c = c_{root} \in C^{(k_{\text{root}})}$, all canonical colorings to $W$ will be generated.

$\text{GENERATE}(c)$
Input: A canonical coloring $c$ with a leading color.
Output: All canonical colorings that are descendants of $c$.
Let $k' := \gamma(c)$;
for each child $k \in Ch(k')$
do
Let $b = b(k)$ be the bottom index of $k$;
for each $b \in \beta(c, b)$
/* Let $Z'$ be a proper subfamily of $Z(c, b)$ */
for each set $Z \in Z'_{c,b}$
do
$\hat{c} := c/Z$;
Let $\hat{c}$ be the canonical coloring
of the set of colorings equivalent to \( \hat{c} \);
Output \( \tilde{c} \);
if \( \tilde{c} \) has a leading color then
\text{Generate}(\tilde{c})
end if
end for
end for
end for

The algorithm can be implemented to run in space polynomial of the size \( p \) of \( W \).

**Theorem 3** Algorithm Generate generates all canonical colorings to \( W \) and can be implemented to run in space polynomial of the size \( p \) and in delay polynomial of the size \( p \).

**Proof.** By Theorem 2, no two colorings \( c/Z \) generated from a coloring \( c \) according to \( \text{Ch}(c) = \bigcup_{k \in \text{Ch}(\gamma(c))} \bigcup_{b \in \beta(c,b(k))} \{c/Z \mid Z \in Z'_{c,b}\} \) are equivalent. To show that no two equivalent colorings will be generated during an execution of algorithm Generate(\( c_{\text{root}} \)), it suffices to show that any coloring \( \hat{c} \) generated from a coloring \( c \) is indeed a child of \( c \), i.e., \( \pi(\hat{c}) = c \). For a canonical coloring \( c \), assume that a coloring \( \hat{c} = c/Z \) is generated by a set \( Z \in Z'_{c,b} \), with an index vector \( k \in \text{Ch}(\gamma(c)) \) and a vector \( b \in \beta(c,b(k)) \). Note that \( Z \subseteq W_1(c) \). Then, by definition of \( c/Z \), each vertex \( w \in W/Z \) satisfies \( c(w) = \hat{c}(w) \); and each vertex \( w \in Z \) satisfies \( c(w) = 1 \) and \( \hat{c}(w) = |c| + 1 \). This means that \( |c| = |\hat{c}| + 1 \) and \( W_{|\hat{c}|} = W_{|c|+1} = Z \). Therefore each vertex \( w \in W_{|\hat{c}|}(\hat{c}) \) satisfies \( c(w) = 1 \) and each vertex \( w \in W \setminus W_{|\hat{c}|}(\hat{c}) \) satisfies \( c(w) = \hat{c}(w) \). Hence \( \pi(\hat{c}) = c \), by definition.

Algorithm Generate can be implemented as a branching procedure for which we only need to keep a work memory. We easily see that each operation in Generate can be implemented in time and space polynomial of \( p = |W| \). To show that Generate can run in delay polynomial of \( p \), it suffices to see that each of the three for-loops in the procedure outputs one of the output.

For any canonical coloring \( c \) with a leading color, the set \( \text{Ch}(\gamma(c)) \) is not empty. We also see that for a given index vector \( k \in \text{Ch}(\gamma(c)) \), the set \( \beta(c,b) \) of vectors is not empty, and that for a vector \( b \in \beta(c,b) \), the family \( Z(c,b) \) is not empty. This means that each of the three for-loops in the procedure is executed at least once, outputing one of the output.

\[ \square \]

3 Results

This section demonstrates how our method is applied to the case where a given graph \( G \) is a chemical graph representing a Naphthalene ring.

3.1 Graph Structure for Naphthalene

Naphthalene is a compound composed of ten carbon atoms, eight of which can be attached by other atom groups. By regarding the carbon atoms in Naphthalene as vertices and the chemical bonds as edges, we get a graph \( G = (V,E) \) with a set \( W \subseteq V \) such that \( V \) corresponds to the set of all carbon atoms in Naphthalene and \( W \) corresponds to the set of the eight carbon atoms that can be substituted by other atom groups. See Fig. 3 for an illustration of graph \( G \) and vertex subset \( W \) for a Naphthalene ring. We see that a graph of Naphthalene has two axial symmetries \( \psi_1 \) and \( \psi_2 \), based on which we denote \( W = \{ w_1, w_2, \ldots, w_8 \} \).

Since \( |W| = 8 \), the set of index vectors \( I_8 \) is given by \( I_8 = \{ k = (k_1, k_2, \ldots, k_8) \mid \sum_{i=1,2,\ldots,8} k_i = 8 \} \), which contains 21 index vectors, as shown in Fig. 4.

3.2 Colorings Types

We show four types of colorings. Fig. 6(a) (resp., (b)-(d)) illustrates a coloring \( c \) of types 0 (resp., 1 to 3). Note that all these four colorings have the same color index \( \gamma(c) = (0, 2, 0, 1, 0, 0, 0, 0) \).

3.3 Canonical Colorings

First we show how to convert an arbitrary coloring to a canonical form. Take the coloring \( c \) of type 0 in Fig. 6(a) as an example, where \( \gamma(c) = (0, 2, 0, 1, 0, 0, 0, 0) \). Denote \( c_{(0)} = c \). We first use three automorphisms \( \psi_1, \psi_2 \) and \( \psi_3 \) to generate all the three colorings \( c_{(i)} \), \( i = 1, 2, 3 \) that are equivalent to \( c_{(0)} \); i.e., \( c_{(1)} = \psi_1[c_{(0)}], c_{(2)} = \psi_2[c_{(0)}] \) and \( c_{(3)} = \psi_3[c_{(0)}] \). See Fig. 7 for these colorings.

We compute the label sequence \( \sigma(c_{(i)}) = (s(W_1(c_{(i)})), s(W_2(c_{(i)})), s(W_3(c_{(i)}))) \) of each coloring \( c_{(i)} \) with \( i = 0, 1, 2, 3 \) as follows:

\[ \sigma(c_{(0)}) = (1, 2, 3, 6, 7, 8, 4, 5), \]
Figure 7: An example of a set of equivalent colorings:
(a) a coloring \( c(0) \); (b) a coloring \( c(1) = \psi_1[c(0)] \) equivalent to \( c(0) \);
(c) a coloring \( c(2) = \psi_2[c(0)] \) equivalent to \( c(0) \); (d) a coloring \( c(3) = \psi_3[c(0)] \) equivalent to \( c(0) \),
where \( c(0) \) is the canonical coloring.

\[
\begin{align*}
\sigma(c(1)) &= (1, 2, 4, 5, 7, 8, 3, 6), \\
\sigma(c(2)) &= (1, 3, 4, 8, 5, 6, 2, 7), \\
\sigma(c(3)) &= (2, 3, 4, 7, 5, 6, 1, 8).
\end{align*}
\]

We see that \( \sigma(c(0)) \) is lexicographically smallest among the four colorings, and therefore \( c(0) \) is the canonical coloring in this equivalence class, in other words, \( c(0) \in C^*(k') \) for \( k' = (0, 2, 1, 0, 0, 0, 0) \).

3.4 Colorings for the Root Index Vector

We start to construct a coloring \( c \) with color index \( \gamma(c) \) equal to the index vector \( k_{\text{root}} = (0, 0, 0, 0, 0, 0, 1). \)

The top and bottom indices of \( k_{\text{root}} \) are given by \( t(k_{\text{root}}) = b(k_{\text{root}}) = 8. \) Clearly the coloring \( c \) is given by \( c(w) = 1 \) for all vertices \( w \in W \), as shown in Fig. 5.

The set of children of index vector \( k_{\text{root}} \) is given by \( \text{Ch}(k_{\text{root}}) = \{(1, 0, 0, 0, 0, 0, 1, 0), (0, 1, 0, 0, 0, 1, 0), (0, 0, 1, 0, 0, 0, 0), (0, 0, 0, 2, 0, 0, 0, 0)\} \).

3.5 Generation of Colorings from Canonical Colorings

We show how a coloring that is a child of a given coloring \( c \) will be constructed by our method described in Section 2.2.4. When a coloring \( c \) and a vector \( b \in B(c, b(k)) \) of \( k = \gamma(c) \) are given, we let \( Z_{c,b}' \) denote the proper subfamily of \( Z(c, b) \) constructed by our method in Section 2.2.4.

As in Section 2.2.4, we distinguish 5 types of a given coloring \( c \).

Case (I). \( c \) is of type 0: As an example, we take the canonical coloring \( c \in C^*(k') \) of type 0 in Fig. 6(a). The leading coloring of \( c \) is 1 and \( W_1(c) = \{w_1, w_6\} \) as shown in Fig. 8(a).

\[
\begin{align*}
\text{Case } (I) &:= \text{Colorings } c/\beta \text{ that are children of the coloring } c \text{ of type 0 in Fig. } 6(a) \text{ for the following vectors } b \in B(c, 2) \text{ and sets } Z \in Z_{c,b}'. \end{align*}
\]

We choose a vector \( b = (1, 0, 0, 1) \) and \( Z = \{w_1, w_6\}; \) \( b = (1, 0, 1, 0) \) and \( Z = \{w_1, w_3\}; \) \( b = (1, 1, 0, 0) \) and \( Z = \{w_2, w_3\}; \) \( b = (0, 1, 1, 0) \) and \( Z = \{w_2, w_6\}; \) \( b = (0, 0, 1, 1) \) and \( Z = \{w_3, w_6\}. \)
Figure 9: Case (II): Colorings \( \hat{c} = c/Z \) with \( Z \in Z'_{b,c} \) for the coloring \( c \) of type 3 in Fig. 6(d) and all vectors \( b \in \beta(c,2) \). (a) \( b = (0,2) \) and \( Z = P_1 = \{w_1, w_4\} \); (b) \( b = (2,0) \) and \( Z = P_2 = \{w_5, w_8\} \); (c) \( b = (1,1) \) and \( Z = \{w_1, w_5\} \); (d) \( b = (1,1) \) and \( Z = \{w_1, w_3\} \).

\( \{w_1, w_5\} \in Z'_{b,c} \) yields a child \( \hat{c} = c/Z \) of the given coloring \( c \), as shown in Fig. 8(a). The other children of \( c \) obtained as \( \hat{c} = c/Z \) by sets \( Z \) in the proper subfamilies \( Z'_{b,c} \) for the rest of the vectors \( b \in \beta(c,2) \) are illustrated in Fig. 8(b)-(f).

Case (II). \( c \) is of type \( h \in \{1,2,3\} \). As an example, we take \( h = 3 \) and the canonical coloring \( c \in C^*(k') \) of type 3 in Fig. 6(d). The leading coloring of \( c \) and \( W_1(c) \) is \( \{w_1, w_4, w_5, w_8\} \). Since \( c \) is of type 3 and is only symmetric with automorphism \( \psi_3 \), the family \( W(c) \) partitioned from the set \( W_1(c) \) is given by

\[
W(c) = \{P_1 = \{w_1, w_4\}, P_2 = P_m = \{w_5, w_8\}\},
\]

where \( m = 2 \). For the index vector \( k' = (0,2,0,1,0,0,0,0) \in I_9 \) equal to \( \gamma(c) \), the top and bottom indices of \( k' \) are \( \ell(k') = \ell = \#|W_1(c)| = 4 \) and \( b(k') = 2 \), and we see that \( \text{Ch}(k') = \{(0,4,0,0,0,0,0,0)\}\).

We take a child \( k = (0,4,0,0,0,0,0,0) \in \text{Ch}(k') \), where the bottom index of \( k \) is \( b = b(k) = 2 \). Then the set \( \beta(c,b(k)) \) with \( b(k) = 2 \) is given by \( \beta(c,2) = \{b = (b_1, b_2) \mid b_1 \in [0,2], i \in [1,2], \sum 1 \leq j \leq 2 b_j = 2\} = \{(2,0),(1,1),(0,2)\} \).

We can generate colorings in \( C(k) \) that are children of \( c \) by assigning color \( |c| + 1 = 4 \) to all vertices in all sets \( Z \in Z'_{b,c} \) for each vector \( b \in \beta(c,2) \). We choose a vector \( b \in \beta(c,2) \). We distinguish the following two subcases (II-a) and (II-b).

(II-a) \( b_i \in \{0,2\} \) for all \( i \in \{1,2,\ldots,m\} \): For vector \( b \in \{(2,0),(0,2)\} \), subfamily \( Z'_{b,c} \) is given by \( Z'_{b,c} = \{u_k, b_k = 2 P_1\}\).

(II-b) \( b_j = 1 \) for some \( j \in \{1,2,\ldots,m\} \): For vector \( b = (1,1) \), fix index \( j = 1 \) and vertex \( s_j = w_1 \in P_1 \) and compute the family \( S = \{S \mid S \in \mathcal{W}_c \cap P_1\} \) \( b_1 = 1 \) for some \( i \in [1,8] \) (see Fig. 5). Note that 1 is the leading color and \( W_1(c) = \{w_1, w_2, \ldots, w_8\} \). Since \( c \) is of type 4 and is symmetric with both \( \psi_1 \) and \( \psi_2 \), the family \( W(c) \) partitioned from the set \( W_1(c) \) is given by

\[
W(c) = \{P_1 = \{w_1, w_2, w_3, w_4\}, P_2 = \{w_5, w_6, w_7, w_8\}\},
\]

where \( m = 2 \). The set of children of \( k_{\text{root}} \) is given by \( \text{Ch}(k_{\text{root}}) = \{(1,0,0,0,0,1,0,0), (0,1,0,0,0,1,0,0), (0,0,1,0,0,0,1,0), (0,0,0,2,0,0,0,0)\}\).

We take a child \( k = (0,0,2,0,0,0,0,0) \in \text{Ch}(k_{\text{root}}) \), where the bottom index of \( k \) is \( b = b(k) = 4 \). Then the set \( \beta(c,b(k)) \) is given by \( \beta(c,4) = \{b = (b_1, b_2) \mid \sum 1 \leq j \leq 2 b_j = 4, 0 \leq b_1, b_2 \leq 4\} = \{(1,3),(3,1),(4,0),(0,4),(2,2)\} \). We can generate all children \( \hat{c} = c/Z \) of \( c \) as \( \hat{c} = c/Z \) for choosing each set \( Z \in Z'_{b,c} \) over all vectors \( b \in \beta(c,2) \).

We choose a vector \( b \in \beta(c,2) \). We distinguish the following three subcases (III-a), (III-b) and (III-c).

(III-a) \( b_j \in \{1,3\} \) for some \( j \in \{1,2,\ldots,m\} \): For vector \( b = (1,3) \), we fix index \( j = i \) and choose a sub-set \( F_i = \{w_1\} \subseteq P_i \) of \( b_i = 1 \) vertex, and compute the family \( S = \{S \mid S \cap P_i \} \) \( b_i = 3 \) by \( \{w_5, w_6, w_8\}, \{w_5, w_7, w_8\}, \{w_6, w_7, w_8\}\}. Therefore, the proper subfamily \( Z'_{b,c} \) is given by \( Z'_{b,c} = \{\{u_1\} \cup S \mid S \subset \mathcal{W}_c \} = \{\{w_1, w_5, w_6, w_8\}, \{w_1, w_5, w_7, w_8\}, \{w_1, w_6, w_7, w_8\}\}. See Fig. 10 for colorings \( \hat{c} = c/Z \) with \( Z \in Z'_{b,c} \) for \( b = (1,3) \).
Figure 11: Case (III-b): The coloring \( \hat{\cdot}c = c/Z \) with \( Z \in Z'_{c,b} \), where \( b = (4,0) \) and \( c \) is given in Fig. 5. In this case, \( Z = \{w_1, w_2, w_3, w_4\} \).

\[
\begin{align*}
\text{(a) type 1} & : \hat{\cdot}c(w)=1 & \text{(b) type 1} & : \hat{\cdot}c(w)=2
\end{align*}
\]

Figure 12: Case (III-c)-(1): The colorings \( \hat{\cdot}c = c/Z \) with \( Z \in Z'_1 \) and \( c \) is given in Fig. 5. (a) \( Z = \{w_1, w_2, w_3, w_5, w_6\} \); (b) \( Z = \{w_1, w_2, w_3, w_7, w_8\} \).

\[
\begin{align*}
\text{(a) type 1} & : \hat{\cdot}c(w)=1 & \text{(b) type 1} & : \hat{\cdot}c(w)=2
\end{align*}
\]

Figure 13: Case (III-c)-(2): The colorings \( \hat{\cdot}c = c/Z \) with \( Z \in Z'_0 \) and \( c \) is given in Fig. 5. (a) \( Z = \{w_1, w_2, w_5, w_7\} \); (b) \( Z = \{w_1, w_3, w_5, w_6\} \); (c) \( Z = \{w_1, w_2, w_5, w_8\} \); (d) \( Z = \{w_1, w_4, w_5, w_8\} \); (e) \( Z = \{w_1, w_3, w_5, w_8\} \); (f) \( Z = \{w_1, w_4, w_5, w_7\} \).

\[
\begin{align*}
\text{(a) type 0} & : \hat{\cdot}c(w)=1 & \text{(b) type 0} & : \hat{\cdot}c(w)=2 \\
\text{(c) type 0} & : \hat{\cdot}c(w)=1 & \text{(d) type 0} & : \hat{\cdot}c(w)=2 \\
\text{(e) type 0} & : \hat{\cdot}c(w)=1 & \text{(f) type 0} & : \hat{\cdot}c(w)=2 
\end{align*}
\]
4 Conclusion

In this paper, we assumed that no vertex in $W$ appear along the axis of any of symmetries $\psi_1$ and $\psi_2$ (i.e., $W \cap Z^1 = W \cap Z^2 = \emptyset$) to design our algorithm for generating colorings to $W$. It is not difficult to modify our algorithm to treat the general case where $W \cap Z^1 \neq \emptyset \neq W \cap Z^2$ so that it runs in polynomial space and polynomial delay. However, the current design of our algorithm heavily depends on the case where the automorphism is determined by exactly two axial symmetries. It is left open to generalize our method to graphs with automorphisms by a set of several axial and rotational symmetries.

References


