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RESONANCE GRAPHS AND A BINARY CODING FOR THE 1-FACTORS OF BENZENOID SYSTEMS*

HEPING ZHANG†, PETER CHE BOR LAM‡, AND WAI CHEE SHIU‡

Abstract. Applying the recently obtained distributive lattice structure on the set of 1-factors, we show that the resonance graphs of any benzenoid systems G, as well as of general plane (weakly) elementary bipartite graphs, are median graphs and thus extend greatly Klavžar et al.'s result. The n-dimensional vectors of nonnegative integers as a labelling for the 1-factors of G with n inner faces are described. The labelling preserves the partial ordering of the above-mentioned lattice and can be transformed into a binary coding for the 1-factors. A simple criterion for such a labelling being binary is given. In particular, Klavžar et al.'s algorithm is modified to generate this binary coding for the 1-factors of a cata-condensed benzenoid system.

Key words. 1-factor, benzenoid system, distributive lattice, resonance graph, Z-transformation graph, binary coding, median graph

AMS subject classifications. 05C70, 05C12, 06D05, 92E10

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1. Introduction.

A hexagonal system is a finite connected plane graph with no cut-vertices in which every interior region is bounded by a regular hexagon of side length 1. A hexagonal system with a 1-factor is regarded as a molecular graph (carbon-skeleton) of a benzenoid hydrocarbon. Hence these kinds of graphs are called *benzenoid systems* and have been extensively investigated; cf. a detailed review [23] due to Randić with the references therein. A benzenoid system is classified into two types: peri-condensed if it has an interior vertex and cata-condensed if it has none. For example, a well-known coronene is peri-condensed, while Dibenz[a,c]anthracene is cata-condensed; both are illustrated in Figure 1.

A 1-factor or perfect matching M of a graph G is a set of pairwise nonadjacent edges (i.e., no two edges share a common endvertex) such that every vertex of G is incident with an edge in M. This graph-theoretical concept coincides with a Kekulé structure of chemical molecules. One research approach is to compute the number of Kekulé structures of a benzenoid system [5]. Another approach is to study individual Kekulé structures and relationships between them. For example, Gutman [10] and Gutman, Teodorović, and Kolaković [11] found different contributions of a leaf and a nonleaf in the tree structure on the set of 1-factors to the resonance energy of a benzenoid hydrocarbon and obtained a more accurate estimate for the resonance energy.

A graph was established on the set of 1-factors of a benzenoid system G: Every 1-factor of G is for a vertex, and a pair of 1-factors is for an edge if they can be transformed into each other by interchanging double and single bonds in an alternating hexagon. This new graph associated with a benzenoid system is called the

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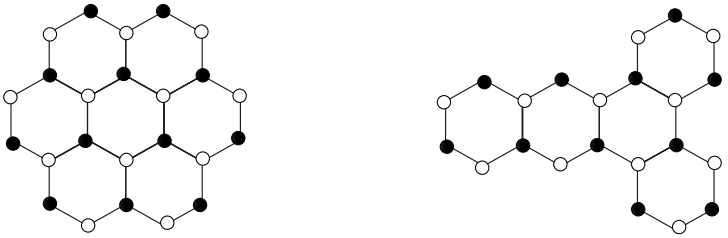

FIG. 1. *Coronene (left) and Dibenz[a,c]anthracene (right).*

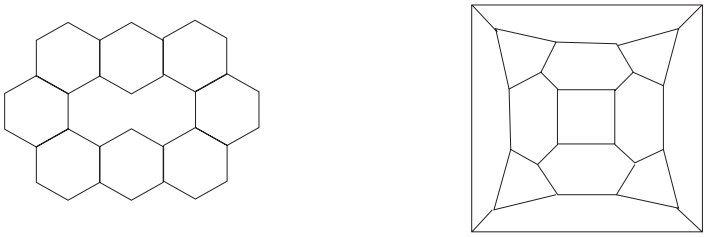

FIG. 2. *A coronoid system (left) and the $B_{12}N_{12}$ fullerene (right).*

Z-*transformation graph* in mathematics by Zhang, Guo, and Chen [28] and the *resonance graph* in chemistry by Randić [22]. Chemical explanation for this concept can be found in [16, 22, 23]. In 1997, Randić [22] showed that the leading eigenvalues (λ) of the resonance graphs correlate with the resonance energy of benzenoids and gave a quite satisfactory regression formula.

For cata-condensed benzenoid systems with n hexagons, Chen and Zhang [2] discovered that the resonance graphs contain Hamilton paths, which can be generated by an algorithm [15]; Randić [22, 23] and Randić et al. [24] showed that some of the resonance graphs can be constructed by proposing a procedure and embedded in n-dimensional Cartesian coordinate grids; Klavžar, Žigert, and Brinkmann [17] proved that the resonance graphs are median graphs. As applications of the latter result, the resonance graphs of cata-condensed benzenoid systems can be isometrically embedded in hypercubes; an algorithm was designed [16] to give each 1-factor a sequence of ones and zeros with length n as a binary coding; a simple method was used to determine the Clar number [18].

Benzenoid systems are a kind of weakly-elementary plane bipartite graphs. In addition, the molecular graphs of most alternate compounds are also plane bipartite graphs. For example, a *coronoid* [4] is a connected subgraph of a hexagonal system such that every edge belongs to at least one hexagon and it contains at least one nonhexagonal interior face (called a corona hole); a boron-nitride (BN) fullerene [3, 8] is a cubic graph embedded on the surface of a sphere so that all faces are (exactly 6) squares and hexagons; see Figure 2. As a unified framework, the resonance graph has already been extended [30, 31, 32] in a natural way on the set of 1-factors of a plane bipartite graph. It was independently shown [7, 33] that the resonance graph of a plane bipartite graph G is connected if and only if G is weakly elementary.

The acyclic orientation of the resonance graph not only enables one to prove [31] that the block graph of the resonance graph of a plane (weakly) elementary bipartite graph G is a path, but also implies a partial ordering on the set of 1-factors of G. Lam and Zhang [20], two of the present authors, showed that this poset associated

with G is a finite distributive lattice by embedding it into an n-dimensional Cartesian coordinate grid with the usual partial ordering, where n is the number of inner faces of G, which implies that each 1-factor is assigned a sequence of nonnegative integers with length n as its labelling.

As applications of the above distributive lattice on the set of 1-factors, in this paper we mainly prove that all connected resonance graphs are median graphs and thus give a significant extension to Klavžar et al.'s result (see Klavžar, Vesel, and Žigert [15], Klavžar et al. [16], Klavžar, Žigert, and Brinkmann [17], Klavžar, Žigert, and Gutman [18]), and we further investigate the labelling for the 1-factors that preserves partial ordering. In the next section, we will introduce the distributive lattice with labelling and give a procedure for generating them. In section 3, by the established distributive lattice structure and the developed techniques, we show that the resonance graph of a plane weakly-elementary bipartite graph is a median graph. In section 4, we give a criterion that such a labelling is a binary coding for all 1-factors of a benzenoid system: it has no coronene as its nice subgraph. In general, the labelling can be transformed into a binary coding so that its length is the diameter of the resonance graph. In section 5, a simple algorithm is designed for generating the binary coding for the 1-factors of a cata-condensed benzenoid system, without producing 1-factors. We conclude this paper with two open problems.

2. Preliminaries and distributive lattices. We now introduce some concepts and notations. A *bipartite* graph means a graph for which every vertex is colored by white or black so that two adjacent vertices receive different colors; such a 2-coloring (white-black) is always given. A bipartite graph G is called *elementary* if G is connected and every edge belongs to a 1-factor of G. For example, coronene, cata-condensed benzenoid systems and boron-nitride fullerenes are plane elementary bipartite graphs.

Let G be a plane bipartite graph with a 1-factor M. A cycle C is *M-alternating* if the edges of C appear alternately in and off the M. An M-alternating cycle C of G is said to be *proper* (*improper*) [30] if every edge of C belonging to M goes from white (black) endvertex to black (white) endvertex by the clockwise orientation of C.

THEOREM 2.1 (see [32]). *A nontrivial plane bipartite graph is elementary if and only if every face is resonant, i.e., every facial boundary is an alternating cycle with some* 1*-factor.*

Elementary components of G mean components of the subgraph obtained from G by removing all fixed single edges (those edges not contained in any 1-factors). G is called *weakly elementary* [19, 25, 32] if every inner face of every elementary component of G is still a face of the original G. For instance, benzenoid systems are these kinds of graphs.

The symmetry difference of finite sets A and B is defined as $A \oplus B := (A \cup B)\backslash(A \cap B)$. This operation can be defined among many finite sets in a natural way and is associative and commutative. If C is an M-alternating cycle of G, then $M \oplus C$ is also a 1-factor, where C may be regarded as its edge-set. It is obvious that a cycle C is proper M-alternating if and only if it is improper $M \oplus C$-alternating. For two 1-factors M and M' of G, $M \oplus M'$ consists of pairwise disjoint M and M'-alternating cycles of G.

A partially ordered set (poset) is a set P with a binary relation $\preceq$ satisfying the reflexivity, antisymmetry, and transitivity. If $x, y \in P$, then we say y covers x if $x \prec y$ and no element z satisfies $x \prec z \prec y$. A poset $(P, \preceq)$ is determined by its covering relation and often denoted by the Hasse diagram. A one-to-one mapping ϕ from P_1 to

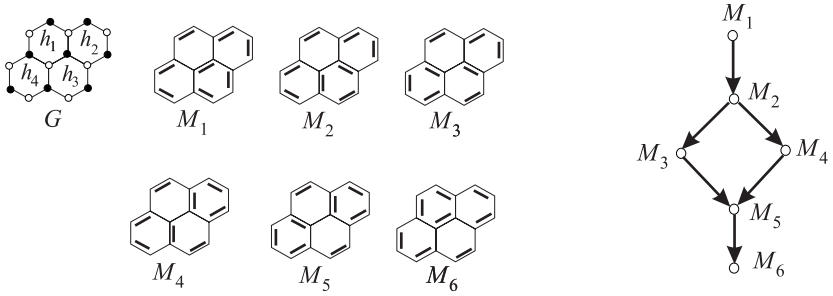

FIG. 3. *Pyrene G, 1-factors M_1 to M_6, and Z-transformation digraph $\vec{Z}(G)$.*

P_2 is an embedding of lattice $(P_1; \vee, \wedge)$ into lattice $(P_2; \vee, \wedge)$ if $\phi(x \vee y) = \phi(x) \vee \phi(y)$ and $\phi(x \wedge y) = \phi(x) \wedge \phi(y)$ for any x and y in P_1. Other terms on posets and lattices used in this paper can be found in [1, 9, 26].

Let G be a plane bipartite graph with a 1-factor. Let $\mathcal{M}(G)$ denote the set of all 1-factors of G and $\mathcal{F}$ the set of all inner faces of G. The *Z-transformation digraph* or *resonance digraph*, denoted by $\vec{Z}(G)$, of 1-factors of G is defined as a digraph on $\mathcal{M}(G)$ such that there exists an arc from M_1 to M_2 provided that $M_1 \oplus M_2$ is a proper M_1- (thus improper M_2-) alternating cycle that is an inner facial boundary of G. Ignoring all directions of arcs of $\vec{Z}(G)$, we get the usual Z-transformation graph or resonance graph, denoted by $Z(G)$.

For example, the Z-transformation digraph of pyrene is constructed in Figure 3. Note that a benzenoid system considered is always drawn so that an edge-direction is vertical and the peaks are colored black (see Figure 1). Accordingly, a proper and an improper alternating hexagon with respect to a 1-factor are the usual proper and improper *sextet*, respectively.

The property that $\vec{Z}(G)$ has no directed cycle implies a partial ordering: $M_1 \preceq M_2$, $M_1, M_2 \in \mathcal{M}(G)$, if and only if $\vec{Z}(G)$ has a directed path from M_2 to M_1. Then $(\mathcal{M}(G), \preceq)$ is a poset. From now on we simply denote it by $\mathcal{M}(G)$.

THEOREM 2.2 (see [20, 29]). *For a plane bipartite graph G, $\vec{Z}(G)$ is the Hasse diagram of $\mathcal{M}(G)$.*

The plane bipartite graph G has a unique 1-factor $M_{\hat{0}}$ such that G has no proper $M_{\hat{0}}$-alternating cycles [30]. Then $M_{\hat{0}}$ is a minimal element of the poset $\mathcal{M}(G)$ and called the *root* 1*-factor* of G. Likely, G has a unique 1-factor $M_{\hat{1}}$ such that G has no improper $M_{\hat{1}}$-alternating cycles. For each $M \in \mathcal{M}(G)$, we define a *function* ϕ_M on $\mathcal{F}$ as follows: For any $f \in \mathcal{F}$, $\phi_M(f)$ is the number of cycles in $M \oplus M_{\hat{0}}$ with f in their interiors. In fact, such cycles are all proper M-alternating and pairwise disjoint if they exist. In particular, $\phi_{M_{\hat{0}}}$ is constantly zero, i.e., every value on the inner faces is 0.

For example, we consider 1-factors $M_{\hat{0}}$ (left) and $M_{\hat{1}}$ (middle) of the coronene in Figure 4. Since $M_{\hat{1}} \oplus M_{\hat{0}}$ consists of two proper $M_{\hat{1}}$-alternating cycles—the boundary and the central hexagon of the coronene (see the rightmost diagram in Figure 4), $\phi_{M_{\hat{1}}}$ is easily computed and represented by the integers indicated in hexagons. As for the pyrene (see Figure 3), the functions ϕ_M of 1-factors $M_1, \ldots, M_6$ are denoted, respectively, by $1111, 1101, 1100, 1001, 1000, 0000$ in such an order of hexagons: h_1, h_2, h_3, h_4.

$\mathbb{Z}^+ = \{0, 1, 2, \ldots\}$ is a linear order with the usual order. $(\mathbb{Z}^+)^{\mathcal{F}}$ is the Cartesian product of $|\mathcal{F}|$ copies of $\mathbb{Z}^+$; each one is indexed by an inner face in $\mathcal{F}$. That is, $(\mathbb{Z}^+)^{\mathcal{F}} = \{(a_1, a_2, \ldots, a_{|\mathcal{F}|})$: each $a_i \in \mathbb{Z}^+$ is indexed by the ith inner face in $\mathcal{F}\}$. It

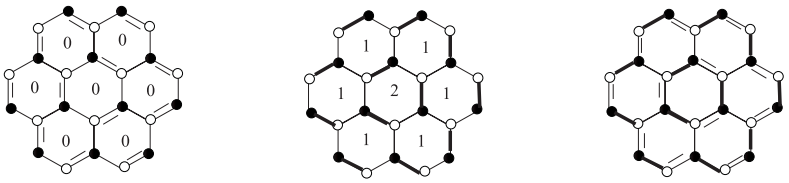

FIG. 4. *Examples of function ϕ_M for the coronene.*

is well known that $(\mathbb{Z}^+)^{\mathcal{F}}$ is an infinite distributive lattice under the usual partial ordering (i.e., for $a, b \in (\mathbb{Z}^+)^{\mathcal{F}}$, $a \leq b$ if and only if $(a)_i \leq (b)_i$ for each $i \in \mathcal{F}$).

In the following, we are given a plane (weakly) elementary bipartite graph G. Each function ϕ_M can be regarded as a vector $\phi_M(\mathcal{F})$ in $(\mathbb{Z}^+)^{\mathcal{F}}$. It was shown in [20] that $\phi : M \mapsto \phi_M$ defines an isomorphism between the poset $\mathcal{M}(G)$ and $\phi(\mathcal{M}(G))$, and the latter is a sublattice of $(\mathbb{Z}^+)^{\mathcal{F}}$.

THEOREM 2.3 (see [20]). *Let G be a plane (weakly) elementary bipartite graph. Then $\mathcal{M}(G)$ is a finite distributive lattice.*

The embedding ϕ of $\mathcal{M}(G)$ into $(\mathbb{Z}^+)^{\mathcal{F}}$ not only enables one to prove the above result, but also gives a labelling for all 1-factors of G. We now turn to discussing a generation of $\mathcal{M}(G)$ with such a labelling.

In obtaining Theorem 2.3, *unit region* and *unit decomposition* of a cycle system $M \oplus M'$ each play a crucial role. For convenience, we now introduce an equivalent form. For $M, M' \in \mathcal{M}(G)$, $\mathcal{C} := M \oplus M'$ consists of pairwise disjoint M and M'-alternating cycles. Let $\psi_{MM'}(f)$ be the number of proper M-alternating cycles in $\mathcal{C}$ with f in their interiors minus the number of improper M-alternating cycles in $\mathcal{C}$ with f in their interiors.

In a sense that $\psi_{MM'}(f)$ here may be allowed to be negative, it is slightly different from the original definition. Accordingly, by Lemmas 4.1 and 4.7 in [20], a relation among the functions $\phi_M, \phi_{M'}$, and $\psi_{MM'}$ can be expressed as follows.

LEMMA 2.4. *For $M, M' \in \mathcal{M}(G)$, $\phi_M - \phi_{M'} = \psi_{MM'}$.*

From the lemma, as a special case we immediately arrive at the following result, which will play an important role in the rest of this paper.

LEMMA 2.5. *For $M, M' \in \mathcal{M}(G)$, M covers M' if and only if $\phi_M(f) - \phi_{M'}(f) = 1$ for $f = f_0$, where f_0 is an inner face bounded by the cycle $M \oplus M'$, and 0 for the other faces in $\mathcal{F}$.*

Based on Theorems 2.2 and 2.3, we can give a generation procedure of lattice $\mathcal{M}(G)$. The main principle is the well-known Jordan–Dedekind theorem in finite distributive lattices: all maximal chains between a pair of elements have the same length. That is, all directed paths between any pair of vertices $\vec{Z}(G)$ are of the same length whenever they exist. Further, Lemma 2.5 also enables one to give the embedding ϕ of $\mathcal{M}(G)$ into $(\mathbb{Z}^+)^{\mathcal{F}}$.

We now describe an outline. First, construct the root 1-factor $M_{\hat{0}}$ and let $\phi_{M_{\hat{0}}} \equiv 0$. The inductive procedure is as follows: Suppose that a 1-factor M and its labelling ϕ_M have been already given. For each improper M-alternating face f_0, $M \oplus f_0$ is another 1-factor covering M, while $\phi_{M \oplus f_0}(f_0) = \phi_M(f_0) + 1$ and the others remain unchanged. Note in the $M \oplus f_0$ operation, f_0 is always regarded as the set of edges bounding the face. A detailed procedure is given as follows.

ALGORITHM 2.6. **Input***: A benzenoid system or plane weakly-elementary bipartite graph G.*
Output*: Lattice $\mathcal{M}$, and labelling list L for all 1-factors of G.*

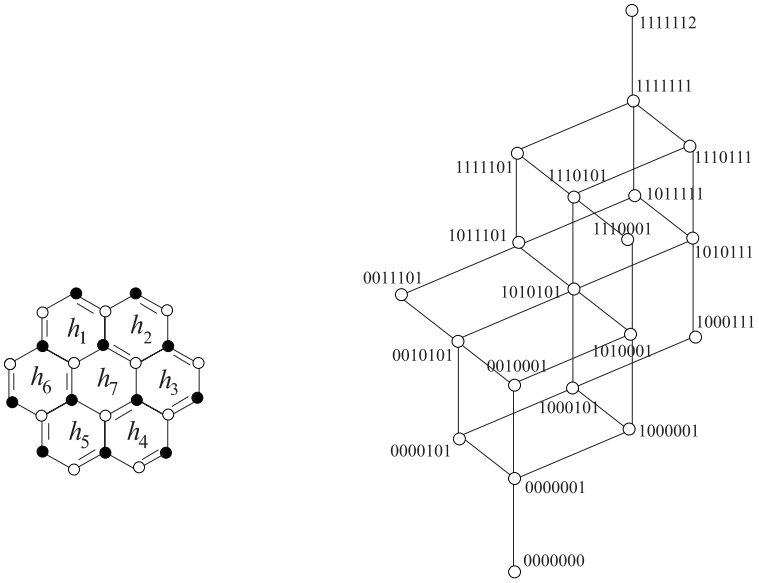

FIG. 5. *The coronene and the distributive lattice on the* 1*-factors with labelling.*

Step 0. *Set* $\mathcal{M} := \emptyset, L := \emptyset$, *and* $i = 0$*; construct the root* 1*-factor* M *of* G *and set* $S_i := \{M\}$ *and* $\phi_M \equiv 0$.
Step 1. *Set* $\mathcal{M} := \mathcal{M} \cup S_i, L := L \cup \{\phi_M : M \in S_i\}$.
Step 2. *If* S_i *has exactly one element* M *and there is no improper* M*-alternating face, stop.*
Step 3. *Set* $S_{i+1} := \{M \oplus f_0 : M \in S_i, f_0$ *is an improper* M*-alternating face of* $G\}$. *For each* $M \oplus f_0$ *in* S_{i+1} *(*$M \oplus f_0$ *covers* M*), compute* $\phi_{M\oplus f_0}$*:* $\phi_{M\oplus f_0}(f_0) := \phi_M(f_0)+1$ *and* $\phi_{M\oplus f_0}(f) := \phi_M(f)$ *for the other faces* f *in* $\mathcal{F}$.
Step 4. *Set* $i := i + 1$*, then go to step* 1.

When this algorithm stops, it also gives the height of $\mathcal{M}(G)$ (it is equal to the diameter of the resonance graph of G; see Corollary 3.5). In fact, S_i consists of all 1-factors with height i. As for step 0, the root 1-factor can be obtained in the following way: First, find any 1-factor of G with the Hungarian algorithm, then repeatedly twist proper alternating inner faces. Finally, we arrive at the root 1-factor. This procedure can be completed in $O(n^2)$ steps, where n is the number of inner faces of G. This is because [29] the height is no more than $\lceil \frac{n(n+2)}{4} \rceil$.

For example, we now implement Algorithm 2.6 to the coronene. The enumeration $h_1, \ldots, h_7$ of its hexagons and the root 1-factor are referred to in Figure 5 (left). When we accomplish the algorithm, the distributive lattice associated with the coronene is produced in Figure 5 (right). For convenience, all of the 1-factors are replaced with their labels. For example, 0000000 corresponds to the root 1-factor, while 1111112 represents the maximum element $M_{\hat{1}}$. In general, the following result shows that such a label can determine uniquely a 1-factor.

PROPOSITION 2.7. *For any given* ϕ_M*, let* $\phi_M \cdot \mathcal{F} := \bigoplus_{f\in\mathcal{F}} \phi_M(f)f$. *Then*

$$M = M_{\hat{0}} \oplus (\phi_M \cdot \mathcal{F}). \tag{1}$$

Proof. $\mathcal{M}(G)$ has a sequence $M_t(= M) \cdots M_0(= M_{\hat{0}})$ such that each M_i covers

M_{i-1} for $1 \le i \le t$. By Lemma 2.5, $M_i \oplus M_{i-1}$ is a proper M_i-alternating face f_i and $\phi_{M_i}(f) - \phi_{M_{i-1}}(f) = 1$ if $f = f_i$, 0, otherwise. That is, $M_i \oplus M_{i-1} = \oplus_{f\in\mathcal{F}}(\phi_{M_i}(f)-\phi_{M_{i-1}}(f))f = (\phi_{M_i}-\phi_{M_{i-1}})\cdot\mathcal{F}$. Hence $M\oplus M_{\hat{0}} = \oplus_{i=1}^{t}(M_i\oplus M_{i-1}) = \oplus_{i=1}^{t}(\phi_{M_i}-\phi_{M_{i-1}})\cdot\mathcal{F} = \sum_{i=1}^{t}(\phi_{M_i}-\phi_{M_{i-1}})\cdot\mathcal{F} = \phi_M\cdot\mathcal{F}$. Here the symmetry difference agrees with addition module 2 and every face $f \in \mathcal{F}$ can be always regarded as the set of edges bounding it. □

Given two labels 1111112 and 1111111, for example, we shall determine their corresponding 1-factors of coronene. For the former, $M_{\hat{0}} \oplus (h_1 \oplus h_2 \oplus h_3 \oplus h_4 \oplus h_5 \oplus h_6 \oplus 2h_7) = M_{\hat{0}} \oplus (h_1 \oplus h_2 \oplus h_3 \oplus h_4 \oplus h_5 \oplus h_6) = M_{\hat{0}} \oplus (C \oplus h_7) = M_{\hat{1}}$, where C denotes the boundary of the coronene. For the latter, $M_{\hat{0}} \oplus (h_1 \oplus h_2 \oplus h_3 \oplus h_4 \oplus h_5 \oplus h_6 \oplus h_7) = M_{\hat{1}} \oplus h_7$.

3. Median graph. Klavžar, Žigert, and Brinkmann [17] showed that the resonance graphs of cata-condensed benzenoid systems, or a subclass of bipartite outplane graphs, are median graphs. By the established distributive lattices and the developed techniques, we now show that the above results hold generally for benzenoid systems, or more general, plane weakly-elementary bipartite graphs G.

Given a connected graph H with vertices u and v, the *interval* $I_H(u, v)$ (or simply $I(u, v)$) between u and v consists of all vertices on shortest paths between u and v. A *median* of vertices u, v, and w is a vertex that lies in $I(u, v) \cap I(u, w) \cap I(v, w)$. A graph is called a *median graph* if every triple of its vertices has a unique median (cf. [12]). We now give the main result of this section as follows.

THEOREM 3.1. *The resonance graph of a plane weakly-elementary bipartite graph G is a median graph.*

To prove the theorem we first give three explicit formulae on distance $d_{Z(G)}(M, M')$, the length of a shortest path between a pair of vertices M and M', in the resonance graph $Z(G)$.

THEOREM 3.2 (distance formula 1). $d_{Z(G)}(M, M') = \sum_{f\in\mathcal{F}} |\phi_M(f) - \phi_{M'}(f)|$.

Proof. Let $P = M_0(= M)M_1 \cdots M_t(= M')$ be a path in $Z(G)$ between M and M'. Then the length

$$\begin{aligned} l(P) = t &= \sum_{i=0}^{t-1}\sum_{f\in\mathcal{F}} |\phi_{M_{i+1}}(f) - \phi_{M_i}(f)| \text{ (by Lemma 2.5)} \\ &= \sum_{f\in\mathcal{F}}\sum_{i=0}^{t-1} |\phi_{M_{i+1}}(f) - \phi_{M_i}(f)| \\ &\ge \sum_{f\in\mathcal{F}} |\sum_{i=0}^{t-1}(\phi_{M_{i+1}}(f) - \phi_{M_i}(f))| \\ &= \sum_{f\in\mathcal{F}} |\phi_M(f) - \phi_{M'}(f)|. \end{aligned} \tag{2}$$

We now choose a special path $P_* := N_s(= M)\cdots N_1N_0N_{-1}\cdots N_{-s'}(= M')$ through the *meet* $N_0 := M \wedge M'$ such that N_i covers N_{i-1} and N_{-j} covers $N_{-(j-1)}$ for all $s \ge i \ge 1$ and $s' \ge j \ge 1$. Recall that $\phi : \mathcal{M}(G) \to \phi(\mathcal{M}(G))$ is an isomorphism and $\phi(\mathcal{M}(G))$ is a sublattice of $(\mathbb{Z}^+)^{\mathcal{F}}$. Then $\phi_{N_0} = \phi_{M\wedge M'} = \phi_M \wedge \phi_{M'}$, and $\phi_{N_0}(f) = \min(\phi_M(f), \phi_{M'}(f))$ for each $f \in \mathcal{F}$. Hence by Lemma 2.5 and similar arguments as above (2) we have that

$$\begin{aligned} l(P_*) = s + s' &= \sum_{f\in\mathcal{F}}(\phi_M(f) - \phi_{N_0}(f)) + \sum_{f\in\mathcal{F}}(\phi_{M'}(f) - \phi_{N_0}(f)) \\ &= \sum_{f\in\mathcal{F}}(\phi_M(f) + \phi_{M'}(f) - 2\phi_{N_0}(f)) \\ &= \sum_{f\in\mathcal{F}}\{\phi_M(f) + \phi_{M'}(f) - 2\min(\phi_M(f), \phi_{M'}(f))\} \\ &= \sum_{f\in\mathcal{F}} |\phi_M(f) - \phi_{M'}(f)| \\ &\le l(P). \end{aligned} \tag{3}$$

This implies that P_* is a shortest path of $Z(G)$ and therefore the theorem holds. ∎

The above distance formula shows that the embedding $\phi : \mathcal{M}(G) \to (\mathbb{Z}^+)^{\mathcal{F}}$ is also distance-preserving.

COROLLARY 3.3 (distance formula 2). $d_{Z(G)}(M, M') = d_{Z(G)}(M \vee M', M \wedge M')$.

Proof. By Theorem 3.2 we have that

$$\begin{aligned} & d_{Z(G)}(M \vee M', M \wedge M') \\ & = \textstyle\sum_{f\in\mathcal{F}}\{\phi_{M\vee M'}(f) - \phi_{M\wedge M'}(f)\} \\ & = \textstyle\sum_{f\in\mathcal{F}}\{\max(\phi_M(f), \phi_{M'}(f)) - \min(\phi_M(f), \phi_{M'}(f))\} \\ & = \textstyle\sum_{f\in\mathcal{F}} |\phi_M(f) - \phi_{M'}(f)| = d_{Z(G)}(M, M'). \end{aligned} \tag{4}$$

∎

Combining Lemma 2.4 with Theorem 3.2, we have the following third formula.

COROLLARY 3.4 (distance formula 3). $d_{Z(G)}(M, M') = \sum_{f\in\mathcal{F}} |\psi_{MM'}(f)|$.

The *height* (or *rank*) of $\mathcal{M}(G)$ is the length of a maximal chain between the greatest and least elements, that is, the length of a directed path of $\vec{Z}(G)$ from the source to sink. Corollary 3.3 shows that $d_{Z(G)}(M_{\hat{0}}, M_{\hat{1}})$ is the diameter (i.e., the largest distance between all pairs of vertices) of $Z(G)$. So we have the following result.

COROLLARY 3.5. *The diameter of $Z(G)$ is equal to the height of $\mathcal{M}(G)$.*

LEMMA 3.6. *For any $M_1, M_2 \in \mathcal{M}(G)$, $I_{Z(G)}(M_1, M_2) = I_{\mathcal{M}(G)}(M_1 \vee M_2, M_1 \wedge M_2)$.*

Proof. For any $M \in \mathcal{M}(G)$, by Theorem 3.2 we have that

$$\begin{aligned} d_{Z(G)}(M_1, M_2) &= \textstyle\sum_{f\in\mathcal{F}} |\phi_{M_1}(f) - \phi_{M_2}(f)| \\ &= \textstyle\sum_{f\in\mathcal{F}} |(\phi_{M_1}(f) - \phi_M(f)) + (\phi_M(f) - \phi_{M_2}(f))| \\ &\le \textstyle\sum_{f\in\mathcal{F}} \{|\phi_{M_1}(f) - \phi_M(f)| + |\phi_M(f) - \phi_{M_2}(f)|\} \\ &= \textstyle\sum_{f\in\mathcal{F}} |\phi_{M_1}(f) - \phi_M(f)| + \sum_{f\in\mathcal{F}} |\phi_M(f) - \phi_{M_2}(f)| \\ &= d_{Z(G)}(M_1, M) + d_{Z(G)}(M, M_2). \end{aligned} \tag{5}$$

Then $M \in I_{Z(G)}(M_1, M_2) \iff$ for all f, $\phi_{M_1}(f) - \phi_M(f)$ and $\phi_M(f) - \phi_{M_2}(f)$ have the same sign $\iff$ for all f, $\min(\phi_{M_1}(f), \phi_{M_2}(f)) \le \phi_M(f) \le \max(\phi_{M_1}(f), \phi_{M_2}(f)) \iff \phi_{M_1\wedge M_2} \le \phi_M \le \phi_{M_1\vee M_2} \iff M_1 \wedge M_2 \preceq M \preceq M_1 \vee M_2$. ∎

Proof of Theorem 3.1. It is sufficient to show that any triple of 1-factors M_1, M_2, and M_3 in $\mathcal{M}(G)$ have a unique median. If M_1, M_2, and M_3 have a median M_0, then by Lemma 3.6 we have that $M_1 \wedge M_2 \preceq M_0 \preceq M_1 \vee M_2, M_2 \wedge M_3 \preceq M_0 \preceq M_2 \vee M_3$ and $M_1 \wedge M_3 \preceq M_0 \preceq M_1 \vee M_3$, which imply that

$$(M_1 \wedge M_2) \vee (M_2 \wedge M_3) \vee (M_1 \wedge M_3) \preceq M_0 \preceq (M_1 \vee M_2) \wedge (M_2 \vee M_3) \wedge (M_1 \vee M_3). \tag{6}$$

Since $\mathcal{M}(G)$ is a distributive lattice (Theorem 2.3), by [1, Theorem 8, Chapter 2] both equalities in (6) hold. This also implies that $(M_1 \wedge M_2) \vee (M_2 \wedge M_3) \vee (M_1 \wedge M_3)$ is a unique median of M_1, M_2, and M_3. ∎

4. Binary coding for the 1-factors. Theorem 3.1 shows that any connected resonance graph is a median graph. Hence it can be isometrically embedded into hypercubes [12]. That is, every 1-factor can be assigned a 0,1-sequence (binary coding) of a given length so that the distance between two 1-factors is equal to the number

of positions for which both of the corresponding sequences differ. In this section, we first give a criterion when ϕ_M itself is such a binary coding for all 1-factors M of a benzenoid system, or a plane weakly-elementary bipartite graph. Then, in a general situation we show how ϕ can be transformed into a binary coding.

Let G be a plane bipartite graph with a 1-factor. A subgraph H of G is said to be *nice* if $G - V(H)$ has a 1-factor. A set S of pairwise disjoint inner faces of G is called a *resonant pattern* of G if G has a 1-factor M such that the boundary of each face in S is an M-alternating cycle. Let $c(G)$ and $k(G)$ denote the numbers of resonant patterns and 1-factors of G, respectively.

LEMMA 4.1 (see [13, 25]). *Let G be a plane bipartite graph with a 1-factor. Then $c(G) \leq k(G)$, and equality holds if and only if G is weakly elementary and for any pair of disjoint cycles that form a nice subgraph, their interiors are disjoint.*

LEMMA 4.2 (see [27]). *For a benzenoid system G, $c(G) = k(G)$ if and only if G has no coronene as its nice subgraph.*

THEOREM 4.3. *Let G be a plane weakly-elementary bipartite graph. Then ϕ is an embedding of $\mathcal{M}(G)$ into $\{0,1\}^{\mathcal{F}}$ if and only if $c(G) = k(G)$; equivalently, for any pair of disjoint cycles that form a nice subgraph their interiors are disjoint.*

Proof. If $\phi_M(f) \geq 2$ for some $M \in \mathcal{M}(G)$ and $f \in \mathcal{F}$, then there exist two disjoint proper M-alternating cycles C_1 and C_2 such that f lies in both interiors of C_1 and C_2. Conversely, suppose that G has a 1-factor M and a pair of disjoint proper M-alternating cycles C_1 and C_2 such that the interior of C_1 is contained in the interior of C_2. Then $M' := M \oplus C_1 \oplus C_2 \in \mathcal{M}(G)$. Since $M \oplus M' = C_1 \cup C_2$, and both C_1 and C_2 are proper M and improper M'-alternating cycles, $\psi_{MM'}(f) = 2$ for any inner face f of G contained in the interior of C_1. By Lemma 2.4, $\phi_M(f) - \phi_{M'}(f) = \psi_{MM'}(f) = 2$. This implies that $\phi_M(f) \geq 2$. Further, the other equivalency is implied by Lemma 4.1. ∎

The following result is an immediate consequence of Lemma 4.2 and Theorem 4.3.

COROLLARY 4.4. *Let G be a benzenoid system. Then ϕ is an embedding of $\mathcal{M}(G)$ into $\{0,1\}^{\mathcal{F}}$ if and only if G has no coronene as its nice subgraph.*

COROLLARY 4.5. *Let G be a benzenoid system. If G has no coronene as its nice subgraph, then the height of $\mathcal{M}(G)$ is equal to the number of resonant hexagons of G.*

Proof. Recall that $M_{\hat{1}}$ is the maximum element of $\mathcal{M}(G)$. Then by distance formula 1 the height $d = \sum_{f \in \mathcal{F}} \phi_{M_{\hat{1}}}(f)$. Since G has no coronene as its nice subgraph, by Corollary 4.4 $\phi_{M_{\hat{1}}}(f) = 0$ or 1 for each $f \in \mathcal{F}$. For a resonant hexagon h, there exists a 1-factor M such that h is proper M-alternating. Further, by Lemma 2.5 we have that $\phi_M(h) - \phi_{M'}(h) = 1$, where $M' := M \oplus h$, which implies that $1 \leq \phi_M(h) \leq \phi_{M_{\hat{1}}}(h) \leq 1$. Hence $\phi_{M_{\hat{1}}}(h) = 1$. But for a nonresonant hexagon h, the $\phi_M(h)$ remain unchanged (zero). Hence d is equal to the number of resonant hexagons of G. ∎

We have already given a criterion that every ϕ_M is a binary coding of M. In a general situation we show how ϕ can be transformed into an embedding $\overline{\phi}$ of $\mathcal{M}(G)$ into Boolean algebra $B_d = \{0,1\}^d$, where $d = \sum_{f \in \mathcal{F}} \phi_{M_{\hat{1}}}(f)$. In fact such an embedding gives a binary coding of length d for all 1-factors of G.

For each $M \in \mathcal{M}(G)$, the function ϕ_M on $\mathcal{F}$ is naturally transformed into the function $\overline{\phi}_M$ on $\mathcal{F}$ as follows: For each $f \in \mathcal{F}$, $\overline{\phi}_M(f)$ is a sequence of length $\phi_{M_{\hat{1}}}(f)$ such that the first $\phi_M(f)$ positions from the left side are all placed 1 and the others 0. Since $0 \leq \phi_M(f) \leq \phi_{M_{\hat{1}}}(f)$, $\overline{\phi}_M(f)$ is well defined. For the coronene, for example, $\phi_{M_{\hat{1}}}(h_7) = 2$ and $\phi_{M_{\hat{1}}}(h_i) = 1 (1 \leq i \leq 6)$. Then $\overline{\phi}_{M_{\hat{1}}}(h_7) = 11$ and $\overline{\phi}_{M_{\hat{1}}}(h_i) = 1 (1 \leq i \leq 6)$ (see Figure 6); while for 1-factor M with $\phi_M = 1111111$, $\overline{\phi}_M(h_7) = 10$ and $\overline{\phi}_M(h_i) = 1 (1 \leq i \leq 6)$.

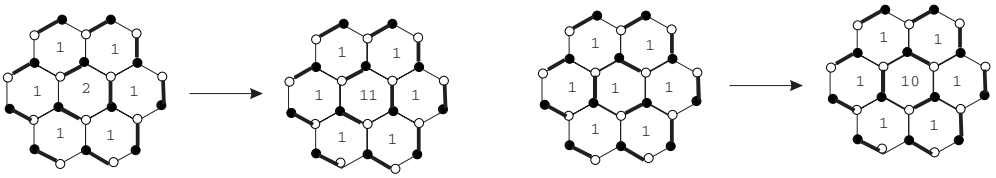

FIG. 6. *The transformation of ϕ_M into a binary coding $\overline{\phi}_M$.*

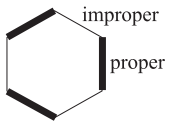

FIG. 7. *Proper and improper positions of a hexagon.*

The following result follows immediately from the property of distance-preserving embedding ϕ.

THEOREM 4.6. *$\overline{\phi} : \mathcal{M}(G) \to \{0,1\}^d$ is a distance-preserving embedding, where d is the height of $\mathcal{M}(G)$.*

5. An algorithm. For a cata-condensed benzenoid system G with d hexagons, there are 2^d different ways by which the resonance graph can be isometrically embedded into a d-hypercube; for example, [15, 16] gave different binary codings. In fact such embeddings are all equivalent under the sense that they can be transformed into each other by permutating the coordinates; though, only ϕ is both order-preserving and distance-preserving embedding. In general, Algorithm 2.6 gives a generation procedure for all ϕ_M. For this special case, we now design a simpler algorithm by modifying Klavžar et al.'s method [16].

If $d \geq 2$, then G has a hexagon that shares exactly one edge with the remainder of G when removing the hexagon. This hexagon corresponds to a monovalency vertex of its inner dual graph (tree). Hence G has a sequence of hexagons $h_1, h_2, \ldots, h_d$, so that each h_j shares one edge (say e_j) with exactly one hexagon (say $h_{a(j)}$) of $h_1, \ldots, h_{j-1}$. We call it a *normal* sequence of hexagons of G.

For a given hexagon, the three thick edges in Figure 7 are said to be in *proper positions*, the other thin edges in *improper positions*. So the common edge of two adjacent hexagons is in a proper position of one hexagon and in an improper position of the other one.

ALGORITHM 5.1. **Input:** *A cata-condensed benzenoid system G with a normal sequence of hexagons $h_1, h_2, \ldots, h_d (d \geq 1)$.*
Output: *A binary coding ϕ for all 1-factors of G: L_d.*
Step 0. $i := 1, L_i := \{0,1\}$.
Step 1. *If $i = d$, stop.*
Step 2. *Let e_{i+1} be the common edge of h_{i+1} with one (say $h_{a(i+1)}$) of $h_1, \ldots, h_i$. If e_{i+1} lies in a proper position of $h_{a(i+1)}$, then set $L_{i+1} := \{x0 : x \in L_i\} \cup \{x1 : x \in L_i$ and $(x)_{a(i+1)} = 1\}$; otherwise, set $L_{i+1} := \{x1 : x \in L_i\} \cup \{x0 : x \in L_i$ and $(x)_{a(i+1)} = 0\}$.*
Step 3. *$i := i + 1$, go to step* 1.

As an example, we implement the algorithm to Dibenz[a,c]anthracene. For a given normal sequence of hexagons $h_1, \ldots, h_5$ (see Figure 8), e_2 and e_3 are in proper

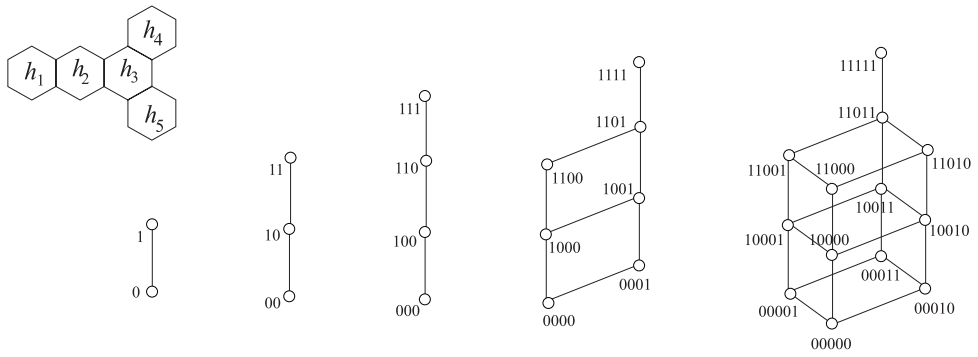

FIG. 8. *An example for implementing Algorithm* 5.1.

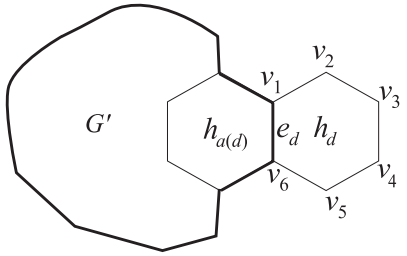

FIG. 9. *Illustration for the proof of Theorem* 5.2.

positions of h_1 and h_2 respectively; both e_4 and e_5 are in improper positions of h_3. Figure 8 illustrates a process of implementing Algorithm 5.1. The binary coding for all of the 1-factors of Dibenz[a,c]anthracene with lattice structure is denoted in the last one. The following theorem gives the correctness of this algorithm.

THEOREM 5.2. *Algorithm* 5.1 *determines the binary coding* ϕ_M *for all* 1*-factors* M *of a cata-condensed benzenoid system* G.

Proof. We proceed by induction on the number d of hexagons of G. If $d = 1$, it is trivial because 1 and 0 correspond to two 1-factors entirely lying in the proper and improper positions of h_1, respectively (see Figure 7).

From now on we suppose that $d \geq 2$. Recall that e_d is the common edge of h_d and some hexagon $h_{a(d)}$. Then $P := h_d - e_d$ is a path of length 5, denoted by $v_1v_2 \cdots v_6$. Let G' be the graph obtained from G by removing the hexagon h_d, i.e., $G' = G - \{v_2, v_3, v_4, v_5\}$; see Figure 9. Then G' has a normal sequence $h_1, \ldots, h_{d-1}$ of hexagons. We claim that the restrictions of all ϕ_M on the hexagons $h_1, \ldots, h_{d-1}$ become the coding $\phi_{\widetilde{M}}$ for all 1-factors $\widetilde{M}$ of G'.

Let $\mathcal{M}_0 := \{M \in \mathcal{M}(G) : \{v_2v_3, v_4v_5\} \subseteq M\}$. For each $M \in \mathcal{M}_0$, $\widetilde{M} := M \setminus \{v_2v_3, v_4v_5\}$ is a 1-factor of G'. This naturally produces a one-to-one correspondence from the 1-factors in $\mathcal{M}_0$ to the 1-factors of G'. For any $M \in \mathcal{M}(G) \setminus \mathcal{M}_0$, $\{v_1v_2, v_3v_4, v_5v_6\} \subseteq M$ and $M \oplus h_d \in \mathcal{M}_0$; by Lemma 2.5 $\phi_M(h_i) = \phi_{M \oplus h_d}(h_i)$ for all $1 \leq i \leq d-1$. Hence the above claim means that

$$\phi_M(h_i) = \phi_{\widetilde{M}}(h_i) \text{ for all } 1 \leq i \leq d-1 \text{ and for all } M \in \mathcal{M}_0. \tag{7}$$

Let $\widetilde{M}_{\hat{0}}$ denote the minimum element of $\mathcal{M}(G')$. It follows that $\phi_{\widetilde{M}_{\hat{0}}\cup\{v_2v_3,v_4v_5\}}(h_i) = \phi_{\widetilde{M}_{\hat{0}}}(h_i) = 0$ for all $1 \le i \le d-1$. If $M_{\hat{0}} = \widetilde{M}_{\hat{0}} \cup \{v_2v_3, v_4v_5\}$, it is trivial. Otherwise, every cycle in $M_{\hat{0}} \oplus (\widetilde{M}_{\hat{0}} \cup \{v_2v_3, v_4v_5\})$ is improper $M_{\hat{0}}$-alternating and thus proper $(\widetilde{M}_{\hat{0}}\cup\{v_2v_3, v_4v_5\})$-alternating. Therefore such a cycle must pass through P; otherwise it is a proper $\widetilde{M}_{\hat{0}}$-alternating cycle in G', a contradiction. Hence such a cycle is unique and denoted by C. In fact $C = h_d$; otherwise, $C + e_d$ contains a proper $\widetilde{M}_{\hat{0}}$-alternating cycle of G', a contradiction. Hence $\widetilde{M}_{\hat{0}} \cup \{v_2v_3, v_4v_5\}$ covers $M_{\hat{0}}$ and $M_{\hat{0}} \oplus h_d = \widetilde{M}_{\hat{0}} \cup \{v_2v_3, v_4v_5\}$. So Lemma 2.5 implies the required result.

For any $M \in \mathcal{M}_0$, by Lemma 2.4 we have

$$\phi_M - \phi_{\widetilde{M}_{\hat{0}}\cup\{v_2v_3,v_4v_5\}} = \psi_{M(\widetilde{M}_{\hat{0}}\cup\{v_2v_3,v_4v_5\})},$$

and

$$\phi_M(h_i) = \psi_{M(\widetilde{M}_{\hat{0}}\cup\{v_2v_3,v_4v_5\})}(h_i) = \psi_{\widetilde{M}\widetilde{M}_{\hat{0}}}(h_i) = \phi_{\widetilde{M}}(h_i) - \phi_{\widetilde{M}_{\hat{0}}}(h_i) = \phi_{\widetilde{M}}(h_i)$$

for all $1 \le i \le d-1$. Claim (7) is verified.

Suppose that Algorithm 5.1 has already determined the binary coding $\phi_{\widetilde{M}}(h_i), 1 \le i \le d-1$, for all 1-factors $\widetilde{M}$ of G'. Hence for each $x \in L_{d-1}$, the corresponding $\widetilde{M} \in \mathcal{M}(G')$ has $\phi_{\widetilde{M}}(h_1, \ldots, h_{d-1}) = x$. For each $M := \widetilde{M} \cup \{v_2v_3, v_4v_5\} \in \mathcal{M}_0$, we have $\phi_M(h_1, \ldots, h_{d-1}) = x$ by the above claim verified.

We now consider the case that e_d is in a proper position of $h_{a(d)}$. Then both v_2v_3 and v_4v_5 are in improper positions of h_d. Therefore $\{v_2v_3, v_4v_5\} \subseteq M_{\hat{0}}$; otherwise, h_d is a proper $M_{\hat{0}}$-alternating, a contradiction. Hence h_d lies outside all cycles in $M \oplus M_{\hat{0}}$. This implies that $\phi_M(h_d) = 0$ and $\phi_M = x0$. Since e_d is always contained in an improper $\widetilde{M}_{\hat{0}}$-alternating cycle, $e_d \notin \widetilde{M}_{\hat{0}}$. This implies that $e_d \in \widetilde{M}$ if and only if e_d is contained in a cycle C in $\widetilde{M}_{\hat{0}} \oplus \widetilde{M}$; that is, $h_{a(d)}$ is contained in the interior of C. If $\phi_{\widetilde{M}}(h_{a(d)}) = 1$, then, equivalently, $e_d \in M$, h_d is an improper M-alternating hexagon and $\phi_{M\oplus h_d} = x1$.

For the other case that e_d is in an improper position of $h_{a(d)}$, analogous arguments can be made. We have that $\phi_M(h_d) = 1$ and $\phi_M = x1$. If $\phi_{\widetilde{M}}(h_{a(d)}) = 0$, then, equivalently, $e_d \in M$, h_d is a proper M-alternating hexagon and $\phi_{M\oplus h_d} = x0$. These conform to step 2 in Algorithm 5.1. Therefore Algorithm 5.1 determines the binary coding ϕ_M for all 1-factors M of G. ∎

Theorem 5.2 shows that the binary coding ϕ_M for the 1-factors M of a catacondensed benzenoid system can be accomplished by Algorithm 5.1. Hence such a binary coding produced by Algorithm 5.1 is independent of its constructive process (i.e., choices for a normal sequence of hexagons) in a sense that each bit corresponds to a specific hexagon. This algorithm is still valid for outplane bipartite graphs.

6. Conclusion. If a plane bipartite graph G is weakly elementary, then from the distributive lattice structure on the 1-factors we know that the resonance graph is a median graph. If G is nonweakly elementary, then we can see that each component of the poset $\mathcal{M}(G)$ is a distributive lattice [29] and each component of the resonance graph is a median graph.

For the weakly-elementary case, the mapping $\phi : \mathcal{M}(G) \to (\mathbb{Z}^+)^{\mathcal{F}}$ is both order-preserving and distance-preserving embedding. When ϕ is transformed into an embedding $\overline{\phi}$ of $\mathcal{M}(G)$ into the Boolean algebra B_d, $\overline{\phi}$ gives an isometric embedding of the resonance graph $Z(G)$ into a d-hypercube—the covering graph of the Boolean

algebra B_d of rank d. Here d is equal to both the height of $\mathcal{M}(G)$ and the diameter of resonance graph $Z(G)$. We conclude by proposing two open problems.

Open problem 1. Determine the smallest integer m such that $\mathcal{M}(G)$ can be embedded into $(\mathbb{Z}^+)^m$. We may conjecture that such smallest integer m is equal to the *resonant number* or *Clar number* in benzenoid systems (i.e., the maximum size of resonant patterns). In Figure 5 we can see that the conjecture is true for the coronene since both smallest m and Clar number are equal to 3, much less than the number 7 of hexagons.

A similar problem was considered recently [6, 14]: If a graph can be isometrically embedded into the m-dimensional integer lattice $\mathbb{Z}^m$ (an infinite graph), then we find such minimum possible dimension m, called the *lattice dimension* of the graph. The lattice dimension of benzenoid systems was determined by Klavžar and Kovše [14] in terms of fundamental trees. Substantially, open problem 1 is to determine the lattice dimension of the resonance graph.

Both embeddings ϕ and $\overline{\phi}$ can be regarded as labellings for the 1-factors, which can be generated by Algorithm 2.6. For the special case of cata-condensed benzenoid system, such two labellings become the same binary coding for all 1-factors, which can be generated by Algorithm 5.1 without involving the generation of all 1-factors; its encoding gives the corresponding 1-factors (see (1)).

Open problem 2. For a general benzenoid system G, how can one design an algorithm to generate the binary coding for all 1-factors, avoiding the generation of $\mathcal{M}(G)$?

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