

Binary Coding of Resonance Graphs of Catacondensed Polyhexes

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(Received January 5, 2023)

Abstract

A catacondensed polyhex H is a connected subgraph of a hexagonal system such that any edge of H lies in a hexagon of H , any triple of hexagons of H has an empty intersection and the inner dual of H is a cactus graph. A perfect matching M of a catacondensed polyhex H is relevant if every cycle of the inner dual of H admits a vertex that corresponds to the hexagon which contributes three edges in M . The vertex set of the graph $\tilde{R}(H)$ consists of all relevant perfect matchings of H , two perfect matchings being adjacent whenever their symmetric difference forms the edge set of a hexagon of H . A labeling that assigns in linear time a binary string to every relevant perfect matching of a catacondensed polyhex is presented. The introduced labeling defines an isometric embedding of $\tilde{R}(H)$ into a hypercube.

1 Introduction

A *benzenoid system* or a *hexagonal system* or simply a *benzenoid* is a finite connected plane graph with no cut vertices in which every interior region is bounded by a regular hexagon. A benzenoid G is *catacondensed* if any triple of hexagons of G has an empty intersection.

A *coronoid* G is a connected subgraph of a hexagonal system such that every edge lies in a hexagon of G and G contains at least one non-hexagon

interior face (called *corona hole*) which should have a size of at least two hexagons. A *polyhex* is either a benzenoid or coronoid. Fig. 1 depicts an example of a catacondensed benzenoid and a (smallest) coronoid.

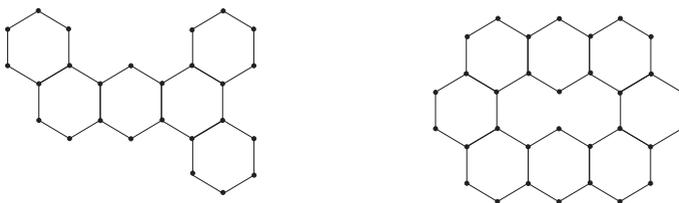


Figure 1. A catacondensed benzenoid (left) and coronoid (right).

In general, coronoids can be regarded as benzenoids with holes. Since benzenoids and coronoids have counterparts in what are called benzenoid and coronoid hydrocarbons, the studies of such systems are of significant chemical relevance [7, 9].

A *matching* of a graph G is a set of pairwise independent edges. A matching is *perfect* if it covers all the vertices of G . In chemistry instead of perfect matchings one speaks of Kekulé structures and the edges contained in a perfect matching are referred to as the double bonds of the respective Kekulé structure. A polyhex that admits at least one Kekulé structure is called *Kekuléan*. Matchings play an important role in chemical graph theory, notable examples are the Hosoya index [18] and the forcing number [32].

The resonance graph was first introduced to model the interaction of two Kekulé structures of aromatic hydrocarbon molecules (that is, perfect matchings of the corresponding graphs) that differ in the position of three double bonds [1, 8, 19]. Formally, the vertex set of the *resonance graph* $R(G)$ of a polyhex G consists of all perfect matchings of G , two perfect matchings being adjacent whenever their symmetric difference is the edge set of a hexagon of G .

Later, the concept was independently re-invented (without any reference to aromatic hydrocarbon molecules) under the name *Z-transformation graph* [29] and extended to elementary plane bipartite graphs (a connected graph is elementary if the union of all perfect matchings forms a connected

subgraph) [30, 31]. Succeeding extensive research showed that resonance graphs of benzenoids, as well as of a plane elementary bipartite graphs possess a lot of structure. In particular, it was established that the resonance graphs of the catacondensed benzenoids belong to the class of median graphs [15]. Furthermore, the resonance graph of every plane elementary bipartite graph G is also median [27] and the set of all perfect matchings of G with a specific partial order is a finite distributive lattice [5, 16].

Some other classes of graphs that admit the concept of resonance graphs are carbon nanotubes [21], fullerenes [22], and catacondensed even ring systems [2].

It turned out that the resonance graphs are associated, somewhat surprisingly, with some other well-known families of graphs. A well-known example are Fibonacci cubes, a class of graphs used in network design, which are precisely the resonance graphs of zigzag benzenoid chains (also known as fibonaccenes) [14]. Later, all plane bipartite graphs with perfect matchings whose resonance graphs are Fibonacci cubes were determined [26]. Moreover, it was also established that none of the Lucas cubes, another class of graphs that can be applied as interconnection topologies, are resonance graphs. Nevertheless, as shown in [34], Lucas cubes are the nontrivial component of the resonance graphs of cyclic polyphenanthrenes. A similar approach was applied in [24] where the so-called matchable Lucas cube was introduced. It is also worth mentioning that resonance graphs of kinky benzenoid systems belong to a class of isometric subgraphs of hypercubes called daisy cubes [33].

Let G be a plane elementary bipartite graph. If H is a subgraph of G obtained by removing a certain face in the periphery of G (a so-called reducible face), then the resonance graph G can be obtained by a peripheral convex expansion from the resonance graph of H [5]. The concept is intrinsically connected with a labeling that establishes an isometric embedding of the resonance graph of a plane elementary bipartite graph (for example, a catacondensed benzenoid graph) into a hypercube [12, 27]. To shed light on the resonance graphs of coronoids, we consider a family of coronoids that can be seen as coronoid counterparts of catacondensed benzenoid graphs in this paper. (Note that a graph H of this family can be

seen as a plane bipartite graph G , where a coronoid hole of H is considered as a face s of G [6]; however, the resonance graph of H cannot be obtained by the above-described decomposition with respect to s because s is not reducible.) Since the resonance graph of a coronoid is not connected in general, we direct our attention to the “main” component of the resonance graph of a coronoid H . That is to say, we study the subgraph of the resonance graph induced by the set of those perfect matchings of H that covers at least one hexagon of each constituent of H .

The paper is organized as follows. In the next section, we define the class of catacondensed polyhexes. Furthermore, we give other definitions, concepts, and results needed in the paper. In Section 3, we introduce the subgraph of the resonance graphs of a catacondensed polyhex H induced by the set of all relevant matchings of H and denoted by $\tilde{R}(H)$. Moreover, we present a recurrence relation in which $\tilde{R}(H)$ of a catacondensed polyhex G with a hexagon h can be expressed as a peripheral expansion defined on $\tilde{R}(H - h)$, where h is either pendant or forms (with other hexagons) a cyclic hexagonal chain. In Section 4, we show that every catacondensed polyhex H admits a sequence of hexagons of H with a property that allows us to label relevant perfect matchings of H in linear time as described in Section 5. It is shown that the introduced labeling defines an isometric embedding of $\tilde{R}(H)$ into a hypercube. Moreover, this result allows us to confirm that $\tilde{R}(H)$ of a catacondensed polyhex H is median.

2 Preliminaries

The vertices of the *inner dual* of a polyhex H , denoted by I_H , are all hexagons of H , two vertices being adjacent if and only if the corresponding hexagons share an edge in H . Note that compared to the usual definition of the inner dual, holes of H are not considered as vertices of I_H . It is easy to see that the inner dual of a catacondensed benzenoid is a tree with a maximum vertex degree equal to three.

A *cactus* graph is a connected graph in which any two simple cycles have at most one vertex in common.

We say that a polyhex H is *catacondensed* if any edge of H lies in a

hexagon of H , any triple of hexagons of H has an empty intersection and the inner dual of H is a cactus graph. An example of a catacondensed polyhex with its inner dual can be seen in Fig. 2.

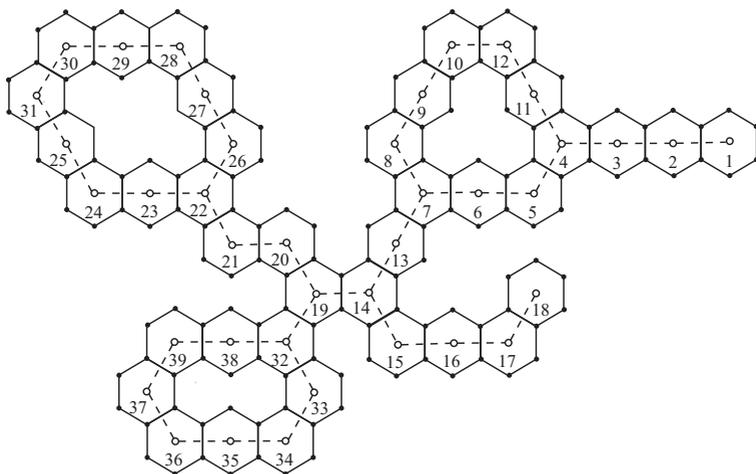


Figure 2. A catacondensed polyhex with its inner dual.

Let h denote a hexagon of a polyhex H . Then $H - h$ denotes a subgraph of H obtained from H by deleting all the vertices and edges of H that belong only to h .

Hexagons h and h' of a polyhex H are *adjacent* if h and h' share an edge. If no hexagon in a catacondensed benzenoid is adjacent to three other hexagons, we say that the graph is a *benzenoid chain*.

Let h be a hexagon of a polyhex H . If h is adjacent to exactly two hexagons, say h' and h'' , such that h' and h'' are not adjacent, then we say that h', h, h'' form a benzenoid chain.

Let L be a subgraph of H induced by a benzenoid chain formed by hexagons h', h, h'' . Hexagon h is *linearly connected* if $L - h' - h''$ is the graph that consists of exactly two isolated vertices, otherwise, we say that h is *angularly connected* (see Fig. 3). If H is composed of two hexagons, then we will say that both hexagons are angularly connected.

A benzenoid chain is called a *fibonaccene* if all of its hexagons, apart from the two terminal ones, are angularly connected.

A graph is *unicyclic* if admits at most one cycle. A catacondensed

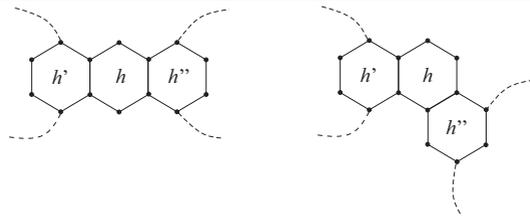


Figure 3. Linearly (left) and angularly (right) connected hexagon h .

polyhex is a *graphene segment* if its inner dual is a unicyclic graph [20]. A graphene segment is a *cyclofusene* if its inner dual is a cycle. A cyclofusene is called a *cyclic fibonaccene* if all of its hexagons are angularly connected.

Let h be a hexagon of a polyhex G . If M is a perfect matching that contains three edges of h , then h is an M -*alternating hexagon*. A perfect matching M of G is *relevant* if every cycle of the inner dual of G admits a vertex that corresponds to an M -alternating hexagon.

Trivially, every perfect matching of a catacondensed benzenoid is relevant, while this is not true for a catacondensed coronoid. As an example observe a perfect matching M of a cyclofusene depicted on the left-hand side of Fig. 4 which does not admit an M -alternating hexagon.

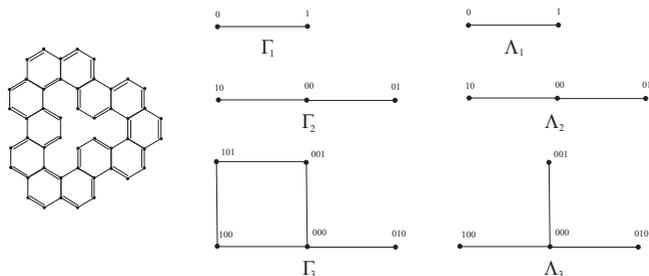


Figure 4. A perfect matching M of a cyclic fibonaccene without an M -alternating hexagon (left); Fibonacci cubes Γ_h and Lucas cubes Λ_h for $h \leq 3$ (right)

For a graph G , let $\tilde{\mathcal{M}}(G)$ be the set of its relevant perfect matchings. For edges e_1, e_2, \dots, e_n of G , let $\tilde{\mathcal{M}}_{e_1, e_2, \dots, e_n}(G)$ denote the set of those relevant perfect matchings of G that contain these edges, while $\tilde{\mathcal{M}}_{\bar{e}}(G)$ denote the set of those relevant perfect matchings of G that do not contain

e .

A hexagon that shares an edge with exactly one other hexagon is called *pendant*. Edges with end-vertices of degree three that belong to a pendant or an angularly connected hexagon will be called *join edges*. Note that a pendant and angularly connected hexagon possess one or two join edges, respectively (see the edge e in the graph on the left-hand side and edges e' and e'' in the graph on the right-hand side of Fig. 5). Let h and h' be adjacent hexagons of a catacondensed polyhex. Then the two edges of h that have exactly one end-vertex in h' are called the *link* of h (to h'). Note for example the links of h depicted in the graph on the right-hand side of Fig. 5.

Let h be a hexagon of a polyhex H . If e is an edge of h with both end-vertices of degree two, then e is an *expandable* edge of H . We say that e is *linearly expandable* if h is a pendant hexagon and e is the edge opposite to the join edge of h . Otherwise, an expandable edge e of h is *angularly expandable*. Fig. 5 shows the expandable edges of two hexagons. Note that the edge e_l (in the graph on the left-hand side) is linearly expandable, while the edges e_a and e'_a are angularly expandable.

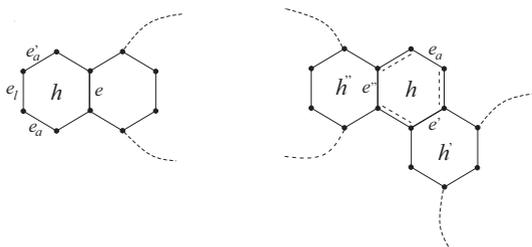


Figure 5. A pendant and angularly connected hexagon.

If x and y are binary strings of equal length, then the *Hamming distance* $H(x, y)$ between x and y is the number of positions in which x and y differ.

The *hypercube* of order h or simply h -*cube*, denoted by Q_h , is the graph $G = (V, E)$ where the vertex set $V(G)$ is the set of all binary strings $u = u_1 u_2 \dots u_h$, $u_i \in \{0, 1\}$, and two vertices $x, y \in V(G)$ are adjacent in Q_h if and only if the Hamming distance between x and y is equal to one.

The *Fibonacci cube* Γ_h , $h \geq 1$, is defined as follows. The vertex set of Γ_h

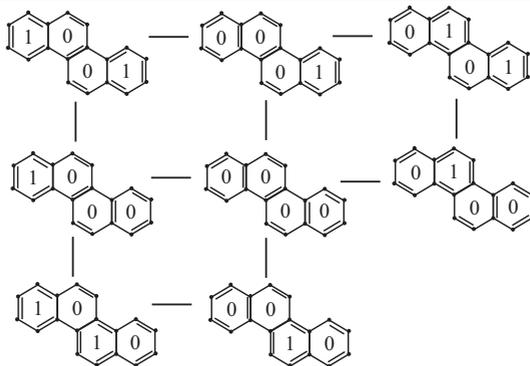


Figure 6. The resonance graph of a fibonaccene with four hexagons

is the set of all binary strings $b_1b_2 \dots b_h$ containing no two consecutive 1s. Two vertices are adjacent in Γ_h if they differ in precisely one bit. Fibonacci cubes are an extensively studied class of graphs, for a comprehensive survey of Fibonacci cubes see [11].

The Fibonacci cube inspired several other families of graphs which can also serve as interconnection topologies. A well-known example is the Lucas cube Λ_h , which is obtained from Γ_h by removing vertices that start and end with 1.

Fibonacci cubes Γ_h and Lucas cubes Λ_h for $h \leq 3$ are depicted on the right-hand side of Fig. 4, while Γ_4 (as the resonance graph of a fibonaccene with four hexagons) can be seen in Fig. 6.

A subgraph H of a graph G is called *convex* if it is connected and if any shortest path of G between vertices of H is already in H . Let H be a fixed subgraph of a graph G . The *peripheral expansion* $\text{pe}(G; H)$ of G with respect to H is the graph obtained from the disjoint union of G and an isomorphic copy of H , in which every vertex of the copy of H is joined by an edge with the corresponding vertex of H . Note that the ends of the newly introduced edges induce a subgraph of $\text{pe}(G; H)$ isomorphic to $H \square K_2$, where $G \square H$ denotes the Cartesian product of graphs G and H , cf. [10]. If H is a convex subgraph of G , then $\text{pe}(G; H)$ is the *convex peripheral expansion* of G with respect to H .

As an example of a peripheral expansion $\text{pe}(G; H)$ observe the graph

in Fig. 6, where G is the graph induced by the set of vertices with labels 1000, 0000, 0100, 1010 and 0010, while H is the graph induced by the set of vertices with labels 1000, 0000, 0100.

If G is a connected graph, then the distance $d_G(u, v)$ (or simply $d(u, v)$) between vertices u and v is the length of a shortest u, v -path, that is, a shortest path between u and v in G .

If G is a graph and $X \subseteq V(G)$, then $G[X]$ denotes the subgraph of G induced by X .

Let $G = (V, E)$ be a graph. A mapping $\phi : V(G) \rightarrow V(Q_h)$ is an *isometric embedding* of G into Q_h if $d_{Q_h}(\phi(u), \phi(v)) = d_G(u, v)$ for every $u, v \in V(G)$. If $u \in V(G)$, we will denote the i -th coordinate of $\phi(u)$ as $\phi(u)_i$.

Graphs that admit an isometric embedding into a hypercube are called *partial cubes*. Note that Fibonacci and Lucas cubes are partial cubes.

We will need the following well-known result (see for example [10]).

Proposition 1. *Let G be a partial cube with an isometric embedding ϕ . If $x, y \in V(G)$ and $\phi(x)_i = \phi(y)_i$, then for every vertex z on a shortest x, y -path it holds that $\phi(z)_i = \phi(x)_i$.*

A median of vertices u, v, w of a graph G is a vertex z that simultaneously lies on a shortest u, v -path, on a shortest u, w -path and on a shortest v, w -path. A graph G is a *median graph* if every triple of its vertices has a unique median.

The following result is shown in [17].

Proposition 2. *A graph is a median graph if and only if it can be obtained from K_1 by a sequence of convex peripheral expansions.*

3 Resonance graphs of catacondensed polyhexes

Let $\tilde{M}(G)$ be the set of relevant matchings of a polyhex G . We will be interested in the subgraph of $R(G)$ induced by $\tilde{M}(G)$ and denoted by $\tilde{R}(G)$.

We already mentioned that every perfect matching of a catacondensed benzenoid is trivially relevant. Thus, if G is a catacondensed benzenoid, we have $\tilde{R}(G) = R(G)$.

Let e be a join edge of a pendant hexagon h of G . Remind that $\tilde{\mathcal{M}}_e(G)$ and $\tilde{\mathcal{M}}_{\bar{e}}(G)$ denote the sets of relevant perfect matchings of G that contain and do not contain e , respectively. Note that the perfect matchings of $\tilde{\mathcal{M}}_{\bar{e}}(G)$ either contain the link of h to its neighboring hexagon or not. We denote the corresponding sets of perfect matchings with $\tilde{\mathcal{M}}_e^\ell(G)$ and $\tilde{\mathcal{M}}_{\bar{e}}^{\bar{\ell}}(G)$, respectively.

It is not difficult to see that the relevant perfect matchings of G can be partitioned as

$$V(\tilde{R}(G)) = \tilde{\mathcal{M}}_e(G) \cup \tilde{\mathcal{M}}_e^\ell(G) \cup \tilde{\mathcal{M}}_{\bar{e}}^{\bar{\ell}}(G).$$

Moreover, if H is the graph obtained from G by removing h , then $\tilde{\mathcal{M}}_e(H)$ and $\tilde{\mathcal{M}}_{\bar{e}}(H)$ one-to-one correspond to $\tilde{\mathcal{M}}_e(G)$ and $\tilde{\mathcal{M}}_{\bar{e}}^{\bar{\ell}}(G)$, respectively.

The following lemma is a generalization of the well-known result for the resonance graph of a catacondensed benzenoid. We skip its proof since it is analogous to the proof presented in [13].

Lemma 1. *Let e be a join edge of a pendant hexagon h of a catacondensed polyhex G . If H is the graph obtained from G by removing h , then $\tilde{R}(G) = \text{pe}(\tilde{R}(H), \tilde{R}(H)[\tilde{\mathcal{M}}_e(H)])$. Moreover, $\tilde{R}(H) = \tilde{R}(G)[\tilde{\mathcal{M}}_e(G) \cup \tilde{\mathcal{M}}_{\bar{e}}^{\bar{\ell}}(G)]$.*

The above lemma presents a recurrence relation for $\tilde{R}(G)$ with respect to $\tilde{R}(G - h)$, where h is a pendant hexagon of a catacondensed polyhex G . Since G may possess a cyclic hexagonal chain as its subgraph, we need a more general result. We first show the following lemma.

Lemma 2. *If M is a relevant perfect matching of a catacondensed polyhex G , then for every link either both edges or none belong to M .*

Proof. Let a link ℓ belongs to a hexagon h of G and let v_h be a vertex of I_G that corresponds to h . Suppose that M contains exactly one edge, say e , of ℓ .

If v_h does not belong to a cycle of I_G , then we can repeat the argument given in [15] as follows. By removing two adjacent end-vertices of

ℓ , we obtain the graph with two connected components, say G_1 and G_2 . Obviously, G_1 and G_2 are both of even order. We may suppose that an end-vertex of e belongs to G_1 . Let G'_1 denote the graph obtained by adding e to G_1 . Obviously, M restricted to G'_1 is a perfect matching of G'_1 . The odd order of G'_1 now yields a contradiction.

Let v_h belong to a cycle C of I_G . If h is M -resonant, the lemma readily follows. Otherwise, since M is relevant, C admits a vertex such that the corresponding hexagon, say h' , is M -resonant. Let e' and e'' denote the join edges of h' . Note that $M \cup \{e', e''\}$ induces a perfect matching on $G - h'$. Since v_h does not belong to a cycle of $I_{G-h'}$, we can then repeat the above argument for $G - h'$ and obtain a contradiction. ■

Let e be an angularly expandable edge of a hexagon h of a catacondensed polyhex G with h' and h'' being hexagons adjacent to h , and let e' (resp. e'') denote the join edge between h and h' (resp. h and h''). Let also ℓ_1, ℓ_2, ℓ' and ℓ'' denote the link from h to h' , from h to h'' , from h' to h and from h'' to h , respectively. Let us denote by $\tilde{\mathcal{M}}_e^{\ell' \vee \ell''}(G)$ the subset of $\tilde{\mathcal{M}}_e(G)$ that contains link ℓ' or link ℓ'' , while $\tilde{\mathcal{M}}_e^{\ell_1, \ell_2}(G)$ denotes the subset of $\tilde{\mathcal{M}}_e(G)$ that contains links ℓ_1 and ℓ_2 .

The following proposition is stated with respect to the above-defined notions.

Proposition 3. *The relevant perfect matchings of a catacondensed polyhex G can be partitioned as*

$$V(\tilde{R}(G)) = \tilde{\mathcal{M}}_{e, e', e''}(G) \cup \tilde{\mathcal{M}}_e^{\ell' \vee \ell''}(G) \cup \tilde{\mathcal{M}}_e^{\ell_1, \ell_2}(G).$$

Proof. Obviously, we have $V(\tilde{R}(G)) = \tilde{\mathcal{M}}_e(G) \cup \tilde{\mathcal{M}}_{\bar{e}}(G)$. Since from Lemma 2 it readily follows that $\tilde{\mathcal{M}}_{\bar{e}}(G) = \tilde{\mathcal{M}}_e^{\ell_1, \ell_2}(G)$ and $\tilde{\mathcal{M}}_e(G) = \tilde{\mathcal{M}}_{e, e', e''}(G) \cup \tilde{\mathcal{M}}_e^{\ell' \vee \ell''}(G)$, the proof is complete. ■

By using Proposition 3 we obtain the following result.

Lemma 3. *Let h be an angularly connected hexagon of a catacondensed polyhex G such that the corresponding vertex in I_G belongs to a cycle of I_G and let H denote the graph obtained from G by removing h . If e is*

the expandable edge of h , while e' and e'' denote the join edges of h , then $\tilde{R}(G) = \text{pe}(\tilde{R}(H), \tilde{R}(H)[\mathcal{M}_{e',e''}(H)])$. Moreover, $\tilde{R}(H) = \tilde{R}(G)[\tilde{\mathcal{M}}_e(G)]$.

Proof. Let h' (resp. h'') denote the hexagon of G adjacent to h that contains e' (resp. e'') and let ℓ_1, ℓ_2, ℓ' and ℓ'' denote the link from h to h' , from h to h'' , from h' to h and from h'' to h , respectively.

Note that H is a catacondensed polyhex. If $M \in \tilde{\mathcal{M}}_e$, then, by Lemma 2 and Proposition 3, either $e' \in M$ or $\ell' \in M$ and either $e'' \in M$ or $\ell'' \in M$. It follows that relevant perfect matchings of $\mathcal{M}_e(G)$ one-to-one correspond to relevant perfect matchings of $\mathcal{M}(H)$. Thus, $\tilde{R}(H) = \tilde{R}(G)[\tilde{\mathcal{M}}_e(G)]$.

Note also that every relevant perfect matching $M \in \mathcal{M}_{e,e',e''}(G)$ is adjacent in $\tilde{R}(G)$ to a unique relevant perfect matching $M' \in \tilde{\mathcal{M}}_e^{\ell_1, \ell_2}(G)$. Moreover, $M_1, M_2 \in \mathcal{M}_{e,e',e''}(G)$ are adjacent in $\tilde{R}(G)[\tilde{\mathcal{M}}_{e,e',e''}(G)]$ if and only if the corresponding relevant perfect matchings $M'_1, M'_2 \in \tilde{\mathcal{M}}_e^{\ell_1, \ell_2}(G)$ are adjacent in $\tilde{R}(G)[\tilde{\mathcal{M}}_e^{\ell_1, \ell_2}(G)]$. It follows that $\tilde{R}(G)[\tilde{\mathcal{M}}_{e,e',e''}(G)]$ and $\tilde{R}(G)[\tilde{\mathcal{M}}_e^{\ell_1, \ell_2}(G)]$ are isomorphic and $\tilde{R}(G) = \text{pe}(\tilde{R}(H), \tilde{R}(H)[\mathcal{M}_{e',e''}(H)])$. ■

4 Normal sequence of hexagons

Let H be a catacondensed benzenoid with n hexagons. A sequence of hexagons h_1, h_2, \dots, h_n of H is called *normal* if for every $i \geq 2$ it holds that h_i is adjacent to exactly one hexagon of h_1, h_2, \dots, h_{i-1} , where $h_{p(i)}, p(i) < i$, denote the hexagon adjacent to h_i . We also state $p(i) = p^1(i)$ and $p^k(i) = p(p^{k-1}(i))$, $k \geq 2$.

It is well known, e.g. [27], that every catacondensed benzenoid H admits a normal sequence of hexagons. Moreover, if h is a hexagon of H we can find in linear time a normal sequence of hexagons h_1, h_2, \dots, h_n such that $h_1 = h$ by applying the breadth-first search from h in I_H (see [12, 27]).

We will generalize the concept of a normal sequence of hexagons for catacondensed polyhexes as follows. Let H be a catacondensed polyhex. A sequence of hexagons h_1, h_2, \dots, h_n of H is called *normal* if

- every cycle C of I_H admits exactly one angularly connected hexagon h_i (called a *cyclic hexagon*) adjacent to exactly two hexagons of

h_1, h_2, \dots, h_{i-1} which both belong to C (these hexagons are denoted by $h_{p(i)}$ and $h_{p^k(i)}$),

- every other hexagon h_i (called an *acyclic hexagon*) is adjacent to exactly one hexagon of h_1, h_2, \dots, h_{i-1} (denoted by $h_{p(i)}$).

Remind that the inner dual I_H of a catacondensed polyhex H is a cactus graph. Clearly, a graph obtained by removing all cycles from a cactus graph consists of connected components which are all trees. Since a connected component obtained by this removal can be seen as a maximal subtree of I_H in this respect, it will be called an *m-tree*. Thus, we may view I_H as a graph composed of *constituents* which are cycles and m-trees.

By the definition of a cactus graph, two cycles of a cactus graph have at most one vertex in common. Nevertheless, since the largest degree of a vertex in the inner dual I_H of catacondensed polyhex H is three, two cycles of I_H cannot admit a common vertex.

Let T_H be a graph whose vertex set consists of all constituents of I_H . Two constituents L and L' are adjacent in T_H if I_H admits an edge $uv \in E(I_H)$ such that $u \in V(L)$ and $v \in V(L')$. Since we can say that u *glues* L with L' , it is called a *g-hexagon* of L . If L is a cycle, then u corresponds to an angularly connected hexagon of H .

Note that I_H admits a so-called tree-like structure which is a well-known property of a cactus graph. Thus, T_H is a tree. More details on the topic can be found in [3], while an example can be seen in Fig. 2 where a graph with five constituents (three cycles and two m-trees) is shown.

By slight modifications of methods presented in [3], T_H can be constructed in linear time. Moreover, since a constituent L of I_H is either a cycle or an m-tree we can find all the g-hexagons and angularly connected hexagons (if H is a cycle) of L within the same time bound. We may also assume that if L is isomorphic to a cycle C , then C is represented as a sequence of hexagons h^1, h^2, \dots, h^k , where h^i is adjacent to h^{i+1} (indices modulo k) for $i = 1, \dots, k$.

In the sequel, we will present a procedure that for a given catacondensed polyhex H (and corresponding I_H and T_H) with n hexagons constructs a normal sequence of hexagons $\mathcal{H} = (h_1, \dots, h_n)$.

As we noted above, every m-tree T (i.e. a corresponding catacondensed benzenoid) admits a normal sequence of hexagons that starts in a hexagon, say \hat{h} , of T . Let then $\text{TREE}(T, k, \ell, \hat{h}, \mathcal{H})$ denotes a procedure that for a m-tree T with k hexagons returns a normal sequence of hexagons $h_{\ell+1}, \dots, h_{\ell+k}$ such that $h_{\ell+1} = \hat{h}$. Moreover, the procedure returns an updated value of ℓ , i.e., $\ell := \ell + k$.

The next procedure returns a normal sequence of hexagons $h_{\ell+1}, \dots, h_{\ell+k}$ for a cycle C of T_H , where $h_{\ell+1}$ is equal to a given hexagon \hat{h} (passed as a parameter).

Procedure $\text{CIRCLE}(C, k, \ell, \hat{h}, \mathcal{H});$

1. Order the hexagons of C in the sequence $h^1, \dots, h^t, \dots, h^k$ such that $h^i h^{i+1} \in E(C)$ (indices modulo k), $h^1 = \hat{h}$, and $h^t (\neq \hat{h})$ is an angularly connected hexagon of C ;
2. **For** $i := 1$ **to** $t - 1$ **do** $h_{\ell+i} := h^i$;
3. **For** $i := t$ **to** k **do** $h_{\ell+i} := h^{k+t-i}$;
4. $\ell := \ell + k$;

end.

Algorithms TREE and CIRCLE are used in the recursive procedure NORMAL that for a given catacondensed polyhex H and the corresponding tree T_H finds a normal sequence of hexagons $\mathcal{H} = (h_1, \dots, h_n)$.

Procedure $\text{NORMAL}(T_H, L, \ell, \hat{h}, \mathcal{H});$

1. Label the constituent L of T_H as discovered;
2. $k :=$ the number of hexagons of L ;
3. **If** L is cycle **then** $\text{CIRCLE}(L, k, \ell, \hat{h}, \mathcal{H})$ **else** $\text{TREE}(L, k, \ell, \hat{h}, \mathcal{H})$;
4. **For every** constituent L' adjacent to L via g-hexagon \hat{h}' of L' **do**
 - 4.1 **If** L' is not discovered **then** $\text{NORMAL}(T_H, L', \ell, \hat{h}', \mathcal{H})$;

end.

Lemma 4. *Every catacondensed polyhex admits a normal sequence of hexagons. Moreover, a normal sequence of hexagons can be found in linear time.*

Proof. Let H be a catacondensed polyhex with n hexagons. As mentioned above, the corresponding tree T_H can be constructed in linear time.

We call the procedure $\text{NORMAL}(T_H, L, \ell, \hat{h}, \mathcal{H})$ such that L is an arbitrary vertex of T_H (a constituent of I_H), $\ell = 0$ and \hat{h} an arbitrary hexagon of L .

If L is an m-tree, then the corresponding subgraph H is a catacondensed benzenoid. Remind that the procedure TREE constructs in linear time a normal sequence of hexagons for a catacondensed benzenoid that starts in an arbitrary hexagon of L . Similarly, if L is a cycle, the procedure CIRCLE performs this task for L within the same time bound. Thus, if L admits k hexagons, the first k hexagons of H are correctly inserted in a normal sequence of hexagons \mathcal{H} in $O(k)$ time.

The procedure NORMAL is then recursively applied for every undiscovered constituent L' of T_H . Since the first hexagon of L' added to \mathcal{H} is the hexagon \hat{h}' which is adjacent to a hexagon of L , say h' , \hat{h}' is adjacent only to h' in \mathcal{H} . Thus, the conditions that define a normal sequence of hexagons are obeyed for every hexagon of L' .

Since T_H is a tree, it follows that \mathcal{H} is a normal sequence of hexagons. Moreover, since every recursive call of NORMAL is performed in time which is linear in the number of hexagons of a constituent of H , the overall time complexity is $O(n)$. ■

Note that for the graph in Fig. 2 an ordering that corresponds to a normal sequence of hexagons is indicated.

5 Labeling

Let h_1, h_2, \dots, h_n be a normal sequence of hexagons of a catacondensed polyhex H and let H_i be the subgraph of H induced by the sequence h_1, h_2, \dots, h_i , e.g. , $H_1 = h_1$ and $H_n = H$.

For a binary string $b = b_1b_2\dots b_n$, let $b0 = b_1b_2\dots b_n0$ and $b1 = b_1b_2\dots b_n1$.

Let L_i , $1 \leq i \leq n$, denote the set of binary strings of length i with

respect to H_i defined as follows.

$$L_1 = \{0, 1\},$$

while for $i \geq 2$ we have $L_i = \{x0 \mid x \in L_{i-1}\} \cup L_{i-1}^\oplus$, where for an acyclic h_i

$$L_{i-1}^\oplus = \{x1 \mid x \in L_{i-1} \text{ and } x_{p(i)} = 1 \text{ (resp. } x_{p(i)} = 0)\},$$

if $h_{p(i)}$ is linearly (resp. angularly) connected;

for a cyclic h_i that is adjacent to both $h_{p(i)}$ and $h_{p^k(i)}$ we have

$$L_{i-1}^\oplus = \{x1 \mid x \in L_{i-1} \text{ and } x_{p(i)} = \alpha \text{ and } x_{p^k(i)} = \beta\},$$

where $\alpha = 1$ (resp. $\alpha = 0$) if $h_{p(i)}$ is linearly (resp. angularly) connected and $\beta = 1$ (resp. $\beta = 0$) if $h_{p^k(i)}$ is linearly (resp. angularly) connected.

We will denote the set L_n for a catacondensed polyhex H with n hexagons also as $L(\tilde{R}(H))$ in the sequel.

Proposition 4. *Let h_1, h_2, \dots, h_n be a normal sequence of hexagons of a catacondensed polyhex H , let H_i be the subgraph of H induced by the sequence h_1, h_2, \dots, h_i and let L_i be the labeling with respect to H_i as defined above. If $n \geq 2$, then*

(i) every $x \in L_i$ corresponds to exactly one perfect matching M_x from $\mathcal{M}(H_i)$,

(ii) if $x, y \in L_i$, then $H(x, y) = 1$ if and only if M_x and M_y are adjacent in $\tilde{R}(H_i)$,

(iii) linearly (resp. angularly) expandable edge $e \in h_j$ of H_i belongs to M_x if and only if $x_j = 1$ (resp. $x_j = 0$).

Proof. As we can see in the left-hand side of Fig. 7, where both catacondensed polyhexes with up to two hexagons and their resonance graphs with corresponding labelings are depicted, the proposition holds for $i = 2$. Let $i > 2$ and let's assume that the proposition holds for i .

Suppose first that h_{i+1} is acyclic.

Let $x \in L_i$. By the induction hypothesis, x corresponds to exactly one perfect matching $M_x \in \mathcal{M}(H_i)$. Moreover, a linearly (resp. angularly)

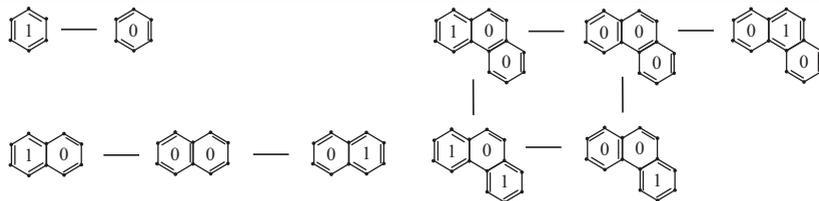


Figure 7. resonance graphs of catacondensed polyhex with one, two, or three hexagons.

expandable edge $e \in h_j$ of H_i belongs to M_x if and only if $x_j = 1$ (resp. $x_j = 0$). Let e denote the common edge between h_{i+1} and $h_{p(i+1)}$.

If e is linearly expandable, then, by the induction hypothesis, $e \in M_x$ if and only if $x_{p(i+1)} = 1$. By Lemma 1, it holds that $\tilde{R}(H_{i+1}) = \text{pe}(\tilde{R}(H_i), \tilde{R}(H_i)[\tilde{\mathcal{M}}_e(H_i)])$ and $\tilde{\mathcal{M}}(H_{i+1}) = \tilde{\mathcal{M}}_e(H_{i+1}) \cup \tilde{\mathcal{M}}_e^\ell(H_{i+1}) \cup \tilde{\mathcal{M}}_e^{\bar{\ell}}(H_{i+1})$.

Since h_{i+1} is acyclic and e is linearly expandable, $L_{i+1} = \{x0 \mid x \in L_i\} \cup \{x1 \mid x \in L_i \text{ and } x_{p(i+1)} = 1\}$. We can see that every $x0 \in L_{i+1}$ corresponds to exactly one perfect matching from the set $\tilde{\mathcal{M}}_e(H_{i+1}) \cup \tilde{\mathcal{M}}_e^{\bar{\ell}}(H_{i+1})$, while every $x1 \in L_{i+1}$ corresponds to exactly one perfect matching from the set $\tilde{\mathcal{M}}_e^\ell(H_{i+1})$. Note that h_{i+1} in H_{i+1} admits exactly one linearly expandable edge (say e_a) and two angularly expandable edges (say e_{l_1} and e_{l_2}). It is clear that a perfect matching from the set $\tilde{\mathcal{M}}_e^\ell(H_{i+1})$ possesses e_a , while a perfect matching from $\tilde{\mathcal{M}}_e(H_{i+1}) \cup \tilde{\mathcal{M}}_e^{\bar{\ell}}(H_{i+1})$, possesses e_{l_1} and e_{l_2} . Thus, every $x0 \in L_{i+1}$ corresponds to a perfect matching that contains two angularly expandable edges, while every $x1 \in L_{i+1}$ corresponds to a perfect matching that contains one linearly expandable edge.

Since it is easy to see that for $y, z \in L_{i+1}$ we have $H(y, z) = 1$ if and only if

a. we can either choose the notation such that $y = x0$ and $z = x1$, $x \in L_i$, or

b. it holds that $y = w\alpha$, $z = w'\alpha$, $\alpha \in \{0, 1\}$, $w, w' \in L_i$, and $H(w, w') = 1$,

the case is settled.

If e is angularly expandable, the proof is analogous.

Finally, suppose that h_{i+1} is a cyclic hexagon adjacent to $h_{p(i+1)}$ and $h_{p^k(i+1)}$. Let e' (resp. e'') denote the join edge of h_{i+1} that belongs to $h_{p(i+1)}$ (resp. $h_{p^k(i+1)}$) and e denote the expandable edge of h_{i+1} . Let also ℓ_1, ℓ_2, ℓ' and ℓ'' denote the link from h to h' , from h to h'' , from h' to h and from h'' to h , respectively.

Note that e' and e'' are linearly or angularly expandable in H_i . Suppose first that e' and e'' are both linearly expandable. By the induction hypothesis, e' and e'' both belong to M_x if and only if $x_{p(i+1)} = 1$ and $x_{p^k(i+1)} = 1$.

We have $\tilde{R}(H_{i+1}) = \text{pe}(\tilde{R}(H_i), \tilde{R}(H_i)[\mathcal{M}_{e',e''}(H_i)])$ and $\tilde{\mathcal{M}}(H_{i+1}) = \tilde{\mathcal{M}}_{e,e',e''}(H_{i+1}) \cup \tilde{\mathcal{M}}_e^{\ell' \vee \ell''}(H_{i+1}) \cup \tilde{\mathcal{M}}_e^{\ell_1, \ell_2}(H_{i+1})$ by Proposition 3 and Lemma 3. Since h_{i+1} is cyclic, while e' and e'' are both linearly expandable, $L_{i+1} = \{x0 \mid x \in L_i\} \cup \{x1 \mid x \in L_i \text{ and } x_{p(i+1)} = 1 \text{ and } x_{p^k(i+1)} = 1\}$. We can see that every $x0 \in L_{i+1}$ corresponds to exactly one perfect matching from the set $\tilde{\mathcal{M}}_{e,e',e''}(H_{i+1}) \cup \tilde{\mathcal{M}}_e^{\ell' \vee \ell''}(H_{i+1})$, while every $x1 \in L_{i+1}$ corresponds to exactly one perfect matching from the set $\tilde{\mathcal{M}}_e^{\ell_1, \ell_2}(H_{i+1})$. Note that e is the only angularly expandable edge of h_{i+1} in H_{i+1} . Thus, every $x0 \in L_{i+1}$ corresponds to a perfect matching that contains e , while every $x1 \in L_{i+1}$ corresponds to a perfect matching that does not contain e .

Since it is easy to see that for $y, z \in L_{i+1}$ we have $H(y, z) = 1$ if and only if

- a. we can either choose the notation such that $y = x0$ and $z = x1$, $x \in L_i$, or
 - b. it holds that $y = w\alpha$, $z = w'\alpha$, $\alpha \in \{0, 1\}$, $w, w' \in L_i$, and $H(w, w') = 1$,
- the case is settled.

The proof for the other three cases (if either e' and e'' are both angularly expandable or exactly one of them is linearly and the other angularly expandable) is analogous. ■

Observe as an example of the described labeling the resonance graph of a cyclofusene with eight hexagons, i.e., $H = H_8$, depicted in Fig. 8. The labeling of $L(\tilde{R}(H_8))$ is obtained with respect to the ordering of hexagons as shown in the graph H bottom right. The left part of the resonance graph represents $\tilde{R}(H - h_8) = \tilde{R}(H_7)$, while the right part shows the

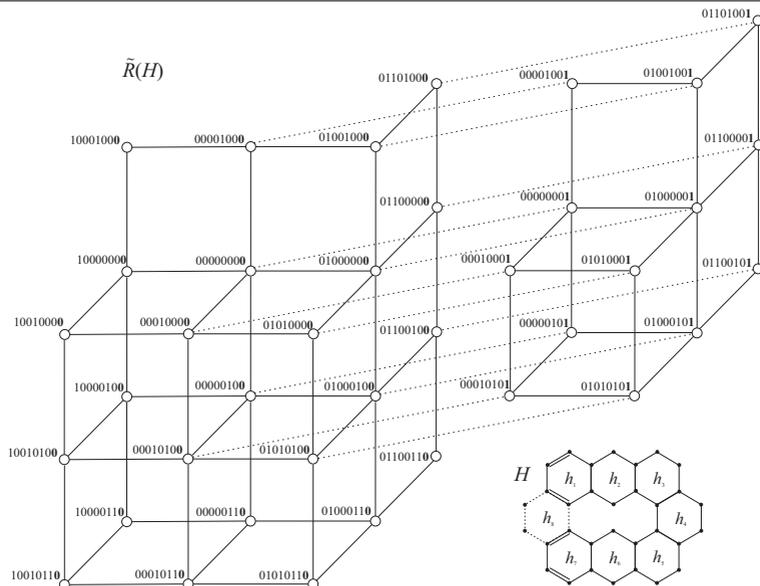


Figure 8. The resonance graph of a cyclofusene with eight hexagons.

subgraph of $\tilde{R}(H_7)$ expanded in the peripheral expansion after h_8 is added to H_7 . The expanded subgraph comprises the vertices of $\tilde{R}(H_7)$ with 0 in the first and seventh position since the relevant perfect matchings that correspond to the expanded subgraph admit both join edges of h_8 , which are also angularly expanded edges of h_1 and h_7 in H_7 . Note that these matchings also contain two other angularly expandable edges of h_1 and h_7 (four edges that are fixed in these matchings are depicted in the figure). It follows that the subgraph of $\tilde{R}(H_7)$ induced by these matchings corresponds to the resonance graph of the subgraph of H induced by the hexagons h_2, \dots, h_6 . Since these hexagons form a fibonaccene with five hexagons, the expanded subgraph is isomorphic to Γ_5 .

Theorem 3.1 from [27] together with [28, Theorem 4.3] indicates that $\tilde{R}(H)$ is a median graph. We use the above-defined labeling to provide proof of this assertion.

We first show that the resonance graph of a catacondensed polyhex is a partial cube.

Theorem 5. *If H is a catacondensed polyhex with n hexagons, then $L(\tilde{R}(H))$ defines an isometric embedding of $\tilde{R}(H)$ into Q_n . Moreover, this embedding can be found in linear time.*

Proof. Let h_1, h_2, \dots, h_n be a normal sequence of hexagons of a catacondensed polyhex H and let H_i be the subgraph of H induced by the sequence h_1, h_2, \dots, h_i . The proof is by induction on i . It is clear that the theorem holds for $i \leq 2$. Let $i > 2$ and let the theorem hold for $i - 1$. Note that every $x \in L_i$ corresponds to exactly one perfect matching $M_x \in V(H_i)$ by Proposition 4. We have to show that for every $x, y \in L_i$ we have $d_{H_i}(M_x, M_y) = H(x, y)$.

Suppose first the h_i is acyclic. If e denote the join edge of h_i , then, since $\tilde{R}(H_i) = \text{pe}(\tilde{R}(H_{i-1}), \tilde{R}(H_{i-1})[\tilde{\mathcal{M}}_e(H_{i-1})])$ and $\tilde{\mathcal{M}}(H_i) = \tilde{\mathcal{M}}_e(H_i) \cup \tilde{\mathcal{M}}_e^\ell(H_i) \cup \tilde{\mathcal{M}}_e^r(H_i)$ by Lemma 1, from the induction hypothesis, it follows that $d_{H_i}(M_x, M_y) = H(x, y)$ if M_x and M_y both belong to $\tilde{\mathcal{M}}_e(H_i) \cup \tilde{\mathcal{M}}_e^\ell(H_i)$. Moreover, since $\tilde{R}(H_{i-1}[\tilde{\mathcal{M}}_e(H_i)])$ is isomorphic to $\tilde{R}(H_i[\tilde{\mathcal{M}}_e^\ell(H_i)])$, we have $d_{H_i}(M_x, M_y) = H(x, y)$ if M_x and M_y both belong to $\tilde{\mathcal{M}}_e^\ell(H_i)$.

We are left to show that $d_{H_i}(M_x, M_y) = H(x, y)$ for every $M_x \in \tilde{\mathcal{M}}_e(H_i) \cup \tilde{\mathcal{M}}_e^\ell(H_i)$ and every $M_y \in \tilde{\mathcal{M}}_e^r(H_i)$. By the definition of the labeling L_i , we have $y = z1$ for some $z \in L_{i-1}$. Note that there exists exactly one perfect matching $M_{y'} \in \tilde{\mathcal{M}}_e(H_i)$ adjacent to M_y . Moreover, the definition of L^i yields $y' = z0$. Since by the induction hypothesis $d_{H_i}(M_x, M_{y'}) = H(x, y') = t$ for some $t \geq 1$, we have $H(x, y) = t + 1$.

As stated in Section 2, $\tilde{R}(H_i)[\tilde{\mathcal{M}}_e(H_i) \cup \tilde{\mathcal{M}}_e^\ell(H_i)]$ is isomorphic to $\tilde{R}(H_i)[\tilde{\mathcal{M}}_e(H_{i-1})] \square K_2$. Remind also that $G \square K_2$ consists of two copies of G , say G^1 and G^2 . It is well-known (see for example [10]) that for $u \in V(G^1)$ and $v \in V(G^2)$ we have $d_{G \square K_2}(u, v) = d_G(u, v') + 1$, where v' is the vertex of $V(G^1)$ adjacent to v . Thus, if $M_x \in \tilde{\mathcal{M}}_e(H_i)$, we have $d_{H_i}(M_x, M_y) = t + 1$ and the case is settled.

Finally, let $M_x \in \tilde{\mathcal{M}}_e^\ell(H_i)$. Since for every $M_y \in \tilde{\mathcal{M}}_e^r(H_i)$, there exists exactly one perfect matching $M_{y'} \in \tilde{\mathcal{M}}_e(H_i)$ adjacent to M_y , a shortest M_x, M_y -path admits a perfect matching, say M_z , from $\tilde{\mathcal{M}}_e(H_i)$. By the induction hypothesis, $d_{H_i}(M_x, M_{y'}) = d_{H_i}(M_x, M_z) + d_{H_i}(M_z, M_{y'}) = H(x, y') = t$. We can conclude from the discussion in the above paragraph that a shortest M_z, M_y -path contains $M_{y'}$. It follows that a shortest

M_x, M_y -path also contains $M_{y'}$. Thus, $d_{H_i}(M_x, M_y) = t + 1$. This assertion completes the proof for an acyclic h_i . Since validation of the theorem for a cyclic h_i is analogous, we are done with the proof of the first part of the theorem.

Remind that Lemma 4 shows that a normal sequence of hexagons of a catacondensed polyhex H can be found in linear time. Since for a given normal sequence of hexagons the corresponding labeling can be clearly found within the same time bound, the proof is complete. ■

Theorem 6. *If H is a catacondensed polyhex, then $\tilde{R}(H)$ is a median graph.*

Proof. Let h_1, h_2, \dots, h_n be a normal sequence of hexagons of a catacondensed polyhex H and let H_i be the subgraph of H induced by the sequence h_1, h_2, \dots, h_i .

The proof is by induction on i . It is clear that the theorem holds for $i \leq 2$. Let $i > 2$ and suppose that the theorem holds for $i - 1$.

Suppose first that h_i is acyclic and let e denote the join edge of h_i . By Lemma 1, we have that $\tilde{R}(H_i) = \text{pe}(\tilde{R}(H_{i-1}), \tilde{R}(H_{i-1})[\tilde{\mathcal{M}}_e(H_{i-1})])$. Thus, by Proposition 2 we have to show that $\tilde{R}(H_{i-1})[\tilde{\mathcal{M}}_e(H_{i-1})]$ is convex in $\tilde{R}(H_{i-1})$. In other words, if $M_x, M_y \in \tilde{\mathcal{M}}_e(H_{i-1}), M_x \neq M_y$, then we have to show that every shortest M_x, M_y -path of $\tilde{R}(H_{i-1})$ is already in $\tilde{R}(H_{i-1})[\tilde{\mathcal{M}}_e(H_{i-1})]$. Let x and y be the labels of L_{i-1} that correspond to M_x and M_y , respectively. Since L_{i-1} is an isometric embedding of $\tilde{R}(H_{i-1})$ into a hypercube, we have $d_{H_{i-1}}(M_x, M_y) = H(x, y) = t > 0$. Suppose that P is a shortest M_x, M_y -path that contains $M_z \in \tilde{\mathcal{M}}_e(H_{i-1})$. By Proposition 4, we have $x_{p(i)} = y_{p(i)} \neq z_{p(i)}$. Thus, from Proposition 1 it follows that P cannot be a shortest M_x, M_y -path and we obtain a contradiction. Since by the induction hypothesis $\tilde{R}(H_{i-1})$ is median, Proposition 2 settles the case.

If h_i is cyclic, the proof is analogous. Let e' (resp. e'') denote the join edge of h_{i+1} that belongs to $h_{p(i+1)}$ (resp. $h_{p^k(i+1)}$) and e denote the expandable edge of h_{i+1} . Let also ℓ_1, ℓ_2, ℓ' and ℓ'' denote the link from h to h' , from h to h'' , from h' to h and from h'' to h , respectively. With respect to Lemma 3, we show that $\tilde{R}(H_{i-1})[\tilde{\mathcal{M}}_{e, e''}(H_{i-1})]$

is convex in $\tilde{R}(H_{i-1})$. Let $M_x, M_y \in \tilde{\mathcal{M}}_{e', e''}(H_{i-1})$, $M_x \neq M_y$, and let x and y be the labels of L_{i-1} that correspond to M_x and M_y , respectively. Since L_{i-1} is an isometric embedding of $\tilde{R}(H_{i-1})$ into a hypercube, we have $d_{H_{i-1}}(M_x, M_y) = H(x, y) = t > 0$. Suppose that P is a shortest M_x, M_y -path that contains $M_z \notin \mathcal{M}_{e', e''}(H_{i-1})$. By Proposition 4, we have $x_{p(i)} = y_{p(i)} = \alpha \in \{0, 1\}$ and $z_{p(i)} \neq \alpha$ or $z_{p^k(i)} \neq \alpha$. Thus, from Proposition 1 it follows that P cannot be a shortest M_x, M_y -path and we obtain a contradiction. By the induction hypothesis, $\tilde{R}(H_{i-1})$ is a median graph. Since $\tilde{R}(H_{i-1})[\tilde{\mathcal{M}}_{e', e''}(H_{i-1})]$ is convex in $\tilde{R}(H_{i-1})$, we can conclude analogously as above that $\tilde{R}(H_i)$ is a median graph. ■

It can be derived from [25, Theorem 3.4 (2)] that the resonance graph of a cyclic fibonaccene with $2n$ hexagons is isomorphic to the Lucas cube of dimension $2n$. (See also the result from [34], which shows that Lucas cubes are the nontrivial component of the resonance graphs of cyclic polyphenanthrenes.) We conclude the paper with the observation that the labeling defined in this section applied on a cyclic fibonaccene gives the set of vertices of the corresponding Lucas cube.

Acknowledgment: This work was supported by the Slovenian Research Agency under the grants P1-0297, J1-2452 and J1-1693.

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