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Fast Computation of Clar Formula for Benzenoid Graphs without Nice Coronenes

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Abstract. A benzenoid system is a finite connected plane graph with no cut vertices in which every interior region is bounded by a regular hexagon of a side length one. Let R be a non-empty set of hexagons of a benzenoid system G. We call R a resonant set of G if the hexagons in R are pairwise disjoint and the subgraph of G obtained by deleting from G the vertices of the hexagons in R has a perfect matching or it is empty. The cardinality of a largest resonant set of a benzenoid system G is said to be its Clar number. A maximum cardinality resonant set of a benzenoid system G or a Clar formula of G is a resonant set whose cardinality is the Clar number of G. We describe a procedure to compute a Clar formula of an elementary benzenoid graph without nice coronenes in linear time.

1 Introduction and preliminaries

A *benzenoid system* or a *benzenoid graph* is a finite connected plane graph with no cut vertices in which every interior region is bounded by a regular hexagon of a side length one.

A benzenoid system can be constructed as follows. Let Z be a circuit on the benzenoid (graphite) lattice. Then a benzenoid system is formed by the vertices and edges of the lattice lying on Z and in the interior of Z. A benzenoid graph G is *catacondensed* if any triple of hexagons of G has empty intersection, otherwise it is *pericondensed*. It is well known that benzenoid graphs possess very natural chemical background. In particular,

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the skeleton of carbon atoms in a benzenoid hydrocarbon is a benzenoid graph. The interested reader is invited to consult the books [4, 5] dedicated to these class of graphs.

A *matching* of a graph G is a set of pairwise independent edges. If a matching covers all the vertices of G, then it is called *perfect*.

Let R be a non-empty set of hexagons of a benzenoid system G. We call R a *resonant set* of G if the hexagons in R are pairwise disjoint and the subgraph of G obtained by deleting from G the vertices of the hexagons in R has a perfect matching or is empty or, equivalently, if the hexagons in R are pairwise disjoint and there exists a perfect matching of G that contains a perfect matching of each hexagon in R. A resonant set is *maximum* if its cardinality is. The cardinality of a maximum resonant set of a benzenoid system G is said to be its *Clar number* and denoted $Cl(G)$. For the convenience, we set $Cl(G) = 0$ if G is empty. A maximum cardinality resonant set (or a *Clar formula*) is a resonant set whose cardinality is the Clar number. As an example see a Clar formula of coronene depicted in the left hand side of Fig. 1.

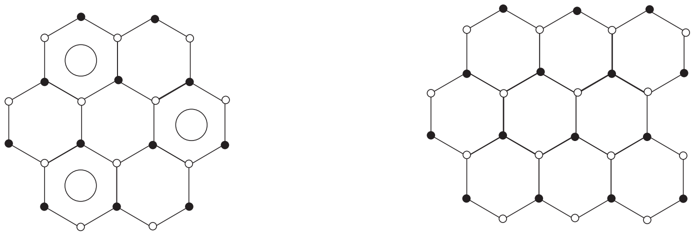

Figure 1: A coronene (left) and a graph without nice coronenes (right).

In chemical graph theory, perfect matchings are called *Kekulé structures*. Analyzing Kekulé structures in general as well as Clar formulas and numbers is of great interest to chemists. In particular, the Clar number is a key concept in the aromatic sextet theory [3].

By solving the Clar problem, we mean obtaining a maximum cardinality resonant set. The Clar problem can be solved in polynomial time using linear programming algorithms [1, 2, 7, 9, 10]. However, no polynomial-time combinatorial algorithm is available for the Clar problem in general, while for some special classes of benzenoid systems with perfect matchings polynomial-time combinatorial algorithms for the Clar problem do exist [6, 14].

The paper is organized as follows. In the sequel of this section we give basic definitions and concepts needed in this paper. In the next section the main result of this paper is presented: a decomposition of an elementary benzenoid graph without nice coronenes G into a system of paths which is based on the 4-tiling of G. In particular, a theorem is given which shows that a path P of this system can always be found. If P is removed from G, then the resulting graph is again an elementary benzenoid graph without nice coronenes with the Clar number $Cl(G) - 1$. Moreover, a hexagon of P that belongs to a maximum cardinality resonant set of G can be found. Using this result, we present in Section 3 an optimal (a linear) algorithm for computing the Clar number and a Clar formula for a graph of this class.

A graph G is called *bipartite* if it is connected and its vertex set can be divided in two disjoint sets V_1 and V_2 such that $V_1 \cup V_2 = V(G)$ and no two vertices from the same set are joined by an edge. Every benzenoid graph G is clearly bipartite, we call vertices of one disjoint set to be *black* and vertices of the other to be *white*.

A *peak* (resp. *valley*) of a benzenoid graph is a vertex that is above (resp. below) all its first neighbors.

A bipartite graph G is called *elementary* if G is connected and every edge belongs to a perfect matching of G. It is well known that if a benzenoid graph G is elementary, then the number of peaks and valleys of G must be equal.

Let P (resp. C) be a path (resp. cycle) in a plane graph G with a perfect matching M. Then P (resp. C) is M-*alternating* if edges of P (resp. C) appear alternately in and off the M.

A face f (finite or infinite) of a plane graph G is said to be *M-resonant* if the boundary of f is an M-alternating cycle with respect to some perfect matching M of G.

Let us call the boundary of the infinite face of G the *outer boundary* or the *outer cycle*.

The symmetry difference of finite sets A and B is defined as $A \oplus B := (A \cup B) \setminus (A \cap B)$. If h is a hexagon of a benzenoid graph G and M a perfect matching of G then in the $M \oplus h$ operation, h is always regarded as the set of edges bounding the hexagon.

A perfect matching M of a bipartite plane graph is said to be *peripheral* if the outer cycle of G is M-alternating.

A subgraph H of a graph G is said to be *nice* if the subgraph of G induced by the set of vertices $V(G) \setminus V(H)$ admits a perfect matching. A benzenoid graph without nice coronenes can be seen in the right hand side of Fig. 1.

Let G be a plane graph. For convenience, we use ∂s to denote the boundary of a finite face s of G, and ∂G to denote the boundary of G, that is, the boundary of the infinite face of G.

Let h denote a hexagon of a benzenoid graph G and P a common path of ∂h and ∂G. Let then $G - h$ denote the resultant subgraph of G by removing the internal vertices and edges of P.

A hexagon h of a benzenoid graph G is *peripheral* if the peripheries of G and f have a nonempty intersection and *internal* otherwise. Let h be a peripheral hexagon of an elementary benzenoid graph G. If $G - h$ is elementary, then we call h a *reducible hexagon* of G. It is well known that an elementary benzenoid graph admits at least two reducible hexagons [11, 15].

Let $h_1, h_2, \ldots, h_k$ denote a sequence of hexagons in an elementary benzenoid graph G. Let $G_i := G_{i-1} - h_i$ for $i = 1, 2, \ldots, k$ and $G_0 := G$. A sequence of hexagons $h_1, h_2, \ldots, h_k$ is said to be *reducible* if h_i is a reducible hexagon in G_{i-1}.

The vertices of the *inner dual* of a benzenoid graph G, denoted by $I(G)$, are the centers of all hexagons of G, two vertices being adjacent if and only if the corresponding hexagons share an edge in G. The inner dual of a benzenoid graph is a subgraph of the regular triangular grid. Clearly, the inner dual of a catacondensed benzenoid graph is a tree with maximum vertex degree three.

An edge e of $I(G)$ is *peripheral*, if e belongs to the infinite face of $I(G)$ and *internal*, otherwise. Analogously, a vertex v of $I(G)$ is *peripheral* if v is the end-vertex of a peripheral edge of $I(G)$ and *internal*, otherwise.

If E' is a subset of edges of a graph G, then let $G \setminus E'$ denote the spanning subgraph of G with the set of edges $E(G) \setminus E'$. Let $I(G)$ be the inner dual of a benzenoid graph G and let S denote a subset of internal edges of $E(I)$. If $I(G) \setminus S$ is the graph where every finite face is a 4-cycle (cf. Figure 2), then S is a *4-tiling* of G. For a 4-tiling S of G we set $I_S(G) := I(G) \setminus S$.

The following theorem shows that the concept of 4-tiling is intrinsically connected with elementary benzenoid graphs.

Theorem 1. *[12] A benzenoid graph G is elementary if and only if G admits a 4-tiling.*

Let G be a pericondensed component of a benzenoid graph and S a 4-tiling of G. The walk in a clockwise direction along the vertices of $I_S(G)$ induces three types of turns. The turns and the corresponding hexagons are denoted $\frac{\pi}{3}$, $\frac{2\pi}{3}$, and $-\frac{\pi}{3}$ in a natural way. A

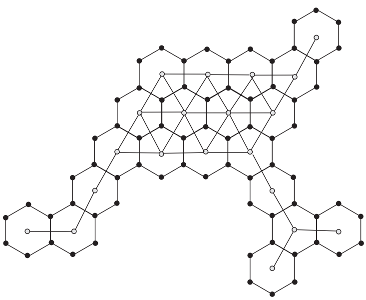

Figure 2: A benzenoid graph with its inner dual (left) and 4-tiling (right).

vertex of $I(G)$ that admits a turn is called a *corner vertex.*

Note also that two edges that belong to the same 4-cycle in $I_S(G)$ and intersect in a common vertex form either a $\frac{2\pi}{3}$ or $\frac{\pi}{3}$ angle. The turns and interior angles of a benzenoid graph are depicted in Figure 3.

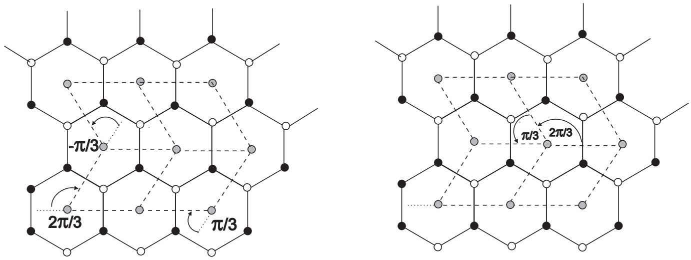

Figure 3: Turns (left) and interior angles (right).

Let G be a benzenoid graph. The subgraph of G that corresponds to the block of the inner dual of G is called a *pericondensed component* of G. By removing the pericondensed components from G we obtain a graph that we call a *catacondensed forest* of G, while its connected component is called a *catacondensed tree.*

A catacondensed tree is called a *link* if it joins the vertices of two pericondensed components and a *beam* otherwise. A graph with one pericondened component and three beams is depicted in Fig 2.

Proposition 1. *[12] A benzenoid graph G is elementary if and only if every pericondensed component of G is elementary.*

Throughout the paper, for a given graph G, let n stand for the number of its vertices.

It is well know that the number of vertices is linear in the number of edges and the number of hexagons of a benzenoid graph.

2 Decomposition

Let H be a pericondensed component of a benzenoid graph G. Note that the boundary of $I(H)$ is a polygon such that its corners correspond to corner vertices of $I(H)$. If $I(H)$ admits only $\frac{\pi}{3}$ and $\frac{2\pi}{3}$ turns, then H is called *convex*.

Proposition 2. *Let H be a convex pericondensed component of an elementary benzenoid graph G. Then the boundary of $I(H)$ is either a quadrangle or a hexagon.*

Proof. Note that a $\frac{2\pi}{3}$ (resp. $\frac{\pi}{3}$) turn induces an interior $\frac{\pi}{3}$ (resp. $\frac{2\pi}{3}$) angle in $I(H)$. It is well known that the sum of the interior angles of a convex n-gon equals $(n-2)\pi$. Since a convex pericondensed component admits only $\frac{\pi}{3}$ and $\frac{2\pi}{3}$ turns, we get

$$(n-2)\pi = (n-x)\frac{2\pi}{3} + x\frac{\pi}{3},$$

where x denote the number of $\frac{2\pi}{3}$ turns in $I(H)$. A straightforward calculation yields $n + x = 6$. Since $n \geq x$, we get $n \in \{3, 4, 5, 6\}$. H is a pericondensed component of an elementary graph, therefore H is also elementary by Proposition 1. It is not difficult to see that every graph with $n = 3$ (resp. $n = 5$) has to be of the shape as depicted in the left (resp. right) hand side of Fig. 4. If $n = 3$, then all three turns of H are $\frac{2\pi}{3}$ turns and H has exactly one peak (resp. valley) and at least two valleys (resp. peaks) and therefore cannot be elementary. Analogously, if $n = 5$, the number of valleys (resp. peaks) exceed the number of peaks (resp. valley) in H by one. It follows that $n \in \{4, 6\}$ and the proof is complete. ∎

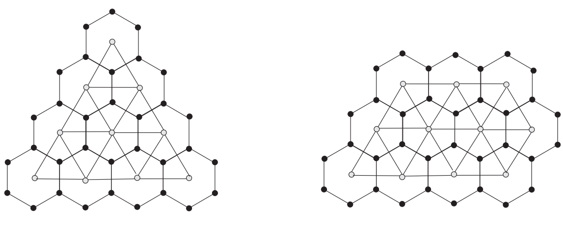

Figure 4: A graph with three $\frac{2\pi}{3}$ turns (left); a graph with five $\frac{\pi}{3}$ turns and one $\frac{2\pi}{3}$ turn (right).

Let M denote a peripheral perfect matching of an elementary benzenoid graph G. Let us define the set of edges $S_M(G)$ as follows: an internal edge h_ih_j of $I(G)$ belongs to $S_M(G)$ if and only if the common edge of the corresponding hexagons h_i and h_j belongs to M.

Theorem 2. *[13] Let M denote a peripheral perfect matching of an elementary benzenoid graph G. Then $S_M(G)$ is a 4-tiling of G.*

Proposition 3. *[13] Let G be an elementary benzenoid graph. Then G admits exactly one 4-tiling if and only if G has no nice coronenes.*

Theorem 3. *[15] Let G be a plane bipartite graph with more than two vertices. Then G is elementary if and only for each face f of G there exists a perfect matching M of G such that f is M-resonant.*

The hexagon of a coronene without peripheral vertices is called the *central hexagon*. If h is a hexagon of an elementary benzenoid graph G, then let $G\backslash h$ denote the graph obtained from G by removing vertices of h.

Lemma 1. *[13] Let H_C denote a coronene which is a nice subgraph of an elementary benzenoid graph G and let h_c denote the central hexagon of H_C. Then $G\backslash h_c$ is elementary.*

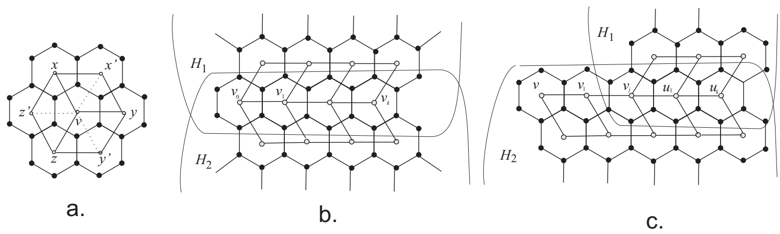

Figure 5: Illustration to the proof of a. Proposition 4, b. Proposition 7, c. Proposition 8

Proposition 4. *Let G be an elementary benzenoid graph with a 4-tiling S. Then G possesses a nice coronene if and only if $I_S(G)$ admits an internal vertex of degree three.*

Proof. Suppose first that G possesses a nice coronene. Let h_c denote the central hexagon of a nice coronene in G. By Lemma 1 the graph $G\backslash h_c$ is elementary. Moreover, it admits a peripheral perfect matching M' by Theorem 3. Let e_1, e_2, e_3 denote three pairwise disjoint edges of h_c. Then $M := M' \cup \{e_1, e_2, e_3\}$ is clearly a peripheral perfect matching in G.

From Theorem 2 it follows that $S_M(G)$ is a 4-tiling in G such that h_c is an internal vertex of degree three in $I_{S_M}(G)$.

Suppose now that G admits an internal vertex v of degree three in $I_S(H)$. Note that the edges of $I_S(H)$ intersecting in v, say vx, vy and wz pairwise form three $\frac{2\pi}{3}$ angles (see Fig. 5a). Let also vx', vy', and vz' be the edges of S. It is easy to see that $S' := S \setminus \{vx', vy', vz'\} \cup \{vx, vy, vz\}$ is a 4-tiling of G. Proposition 3 now yields the assertion. ■

Corollary 1. *If G is an elementary benzenoid graph without nice coronenes and h its reducible hexagon, then $G - h$ is an elementary benzenoid graph without nice coronenes.*

Let I' be a subgraph of the inner dual of a benzenoid graph. A path P of I' with the property that every two edges of P lie on the same line is called a *straight path*. A straight path P is said to be *peripheral* if every hexagon of P is peripheral.

Let G be an elementary benzenoid graph with a 4-tiling S. Let $v = v_0$ be a peripheral vertex of a pericondensed component such that $d_{I_S(G)}(v) \geq 3$ and v_0v_1 an the internal edge of $I_S(G)$. An *internal path* $P_v = v_0, v_1, \ldots, v_k$ corresponding to v is the maximal straight path in $I_S(G)$ that contains v_0v_1 (see Fig. 5b).

Proposition 5. *Let G be an elementary benzenoid graph without nice coronenes. Then the periphery of the inner dual of a convex pericondensed subgraph of G is a parallelogram.*

Proof. Let S denote a 4-tiling of G and H a convex pericondensed subgraph of G. Note that H is elementary by Proposition 1 (since it admits a 4-tiling) and set $I_S(H) := I(H) \setminus S$.

Suppose first that H admits only $\frac{\pi}{3}$ turns. From the proof of Proposition 2 then it follows that the periphery of $I(H)$ is a hexagon. We will show that $I_S(H)$ has to admit an internal vertex of degree three. Note first that $I_S(H)$ admits three corner vertices of degree two (the corresponding edges form one $\frac{2\pi}{3}$ angle) and three corner vertices of degree three (the corresponding edges form two $\frac{\pi}{3}$ angles). If v is a corner vertex of degree three, let then $P_v = v_0, v_1, \ldots, v_k$ be the internal path corresponding to $v = v_0$. Since every face of $I_S(G)$ is a 4-cycle, the vertex v_i has to be of degree four in $I_S(G)$ for every $i = 1, \ldots, k-1$ (see Fig. 5b). Since P_v is maximal with respect to the line determined by v_0v_1, the vertex v_k has to be of degree three in $I_S(G)$. Moreover, v_k has to be internal, since otherwise $I(H)$ would admit a $-\frac{\pi}{3}$ turn contradicting the convexity of H. Since we showed that H admits an internal vertex of degree three, from Proposition 4 then it follows that H has a nice coronene and we obtain a contradiction.

We have shown above that H has to admit a $\frac{2\pi}{3}$ turn. Moreover, H has to admit a $\frac{\pi}{3}$ turn since otherwise the number of peaks and valleys in H cannot be equal. Since the sum of turns of $I(H)$ must equal 2π, it follows that H has to admit exactly two $\frac{\pi}{3}$ turns and exactly two $\frac{2\pi}{3}$ turns. This observation concludes the proof. ■

Let G be a benzenoid graph with a 4-tiling S and h be a peripheral hexagon of G. The hexagon h is called *removable* if h admits a $\frac{\pi}{3}$ turn and the corresponding vertex in $I_S(G)$ is of degree two, or h admits a $-\frac{\pi}{3}$ turn and the corresponding vertex in $I_S(G)$ is of degree three.

Proposition 6. *If G is an elementary benzenoid graph without nice coronenes, then h is a reducible hexagon of G if and only if h is either removable or h is of degree one.*

Proof. Suppose first that h belongs to a catacondensed forest of G. It is easy to see that h is reducible if and only if h is of degree one.

If h belongs to a pericondensed component of G, then the 'if' part of the proposition follows from Theorem 1, while the 'only if' part follows from Proposition 3. ■

Proposition 7. *Let H be a pericondensed component of an elementary benzenoid graph G without nice coronenes. Then $I(H)$ admits at least two $\frac{2\pi}{3}$ turns.*

Proof. If H is convex, then the periphery of $I(H)$ is parallelogram by Proposition 5 and the assertion follows.

Assume then that H is not convex. Since H is not convex, it admits at least one $-\frac{\pi}{3}$ turn. Clearly, H also admits $\frac{2\pi}{3}$ or $\frac{\pi}{3}$ turns.

If H does not admit a $\frac{\pi}{3}$ turn, let then x and y denote the number of $-\frac{\pi}{3}$ and $\frac{2\pi}{3}$ turns, respectively. From $x(-\frac{\pi}{3}) + y\frac{2\pi}{3} = 2\pi$ we get $2y - x = 6$. It is easy to see that y must be greater than four and the assertion follows. (In fact, y must be at least six in order to construct an elementary benzenoid graph.)

Assume then that H admits at least one $\frac{\pi}{3}$ turn. Let S denote the 4-tiling of H. The rest of the proof is by induction on the number of 4-cycles in $I_S(H)$. If $I_S(H)$ admits exactly two 4-cycles, the claim is obvious. Suppose that the claim does not hold and let H denote a pericondensed component of G with the least number of 4-cycles, such that H admits at most one $\frac{2\pi}{3}$ turn. Since H is elementary, from Theorem 1 and Proposition 6 it follows that H admits a removable hexagon.

We distinguish the following two cases:

A. H admits a $\frac{\pi}{3}$ turn such that the corresponding vertex v in $I_S(H)$ is of degree at least three. Let then $P_v = v, v_1, \ldots, v_k$ be an internal path corresponding to v. Since every face of $I_S(G)$ is a 4-cycle, v_i has to be of degree four in $I_S(H)$ for every $i = 1, \ldots, k-1$. Since P_v is maximal with respect to the line determined by v_0v_1, the vertex v_k has to be of degree three in $I_S(G)$. Moreover, v_k has to admit a $-\frac{\pi}{3}$ turn by Proposition 4. Both v_0 and v_k are peripheral, therefore P_v partition H into two subgraphs, say H_1 and H_2, such that the hexagons of P_v form the intersection of H_1 and H_2 (see Fig. 5b). Since both H_1 and H_2 admit a 4-tiling, they are both elementary. Moreover, v induces a $\frac{2\pi}{3}$ turn in both H_1 and H_2. Since H admits at most one $\frac{2\pi}{3}$ turn, we may assume w.l.o.g. that H_1 admits at most one $\frac{2\pi}{3}$ turn and we obtain a contradiction because of the minimality of H.

B. H admits a $\frac{\pi}{3}$ turn such that the corresponding vertex v in $I_S(H)$ is of degree two. Note that v is reducible in H. Let uv denote the edge of S in $I_S(H)$ and set $H' := H - v$. From Proposition 4 it follows that u cannot be of degree three in $I_S(H')$. If u is not a cut-vertex (i.e. H' is composed of exactly on pericondensed component), then H' and H admit the same number of $\frac{2\pi}{3}$ turns and we get a contradiction because of the minimality of H. If u is a cut-vertex, then u is the only common vertex of two elementary pericondensed components, say H_1 and H_2, and we obtain a contradiction analogously as in case A.

Since we examined all possible cases, the proof is complete. ■

Let G be an elementary pericondensed benzenoid graph without nice coronenes and S the 4-tiling of G. If $u \in V(I(G))$ is a vertex of degree one in $I(G)$, then the maximal straight path $P_u = u_0, u_1, \ldots, u_k$ in the catacondensed forest of $I(G)$ is called a *straight beam.*

Let $P_u = u_0, u_1, \ldots, u_k$ be a straight beam:

If u_k is a vertex of degree three such that it belongs to two distinct straight beams, then $P'_u = u_0, u_1, \ldots, u_{k-1}$ is called a *straight beam of type 1* or SBT1.

If u_k is a vertex of degree two, then $P_u = u_0, u_1, \ldots, u_k$ is called a *straight beam of type 2* or SBT2.

If u_k is adjacent to a peripheral vertex v of degree three in $I_S(G)$ which admits a $\frac{\pi}{3}$ turn in a pericondensed component of G, then $P'_u = u_0, u_1, \ldots, u_k, v$ is called a *straight beam of type 3* or SBT3.

If v is a peripheral vertex of $I(G)$ which admits a $\frac{2\pi}{3}$ turn in a pericondensed component of G, then a maximal peripheral straight path $P_v = u_1, \ldots, u_i, v, v_1, \ldots, v_j$ where u_1 is of degree one is called a *peripheral path.* Note that the subpath $u_1, \ldots, u_i$ is empty if

$d_{I_S(G)}(v) = 2$. If the subpath $u_1, \ldots, u_i$ is not empty (i.e. $d_{I_S(G)}(v) = 3$), then a peripheral path is called an *extended peripheral path*.

Let v be a peripheral vertex of degree two in $I(G)$ which admits a $\frac{2\pi}{3}$ turn. Then two peripheral paths with the common vertex v compose a *peripheral twin path* with a *critical point* v.

If a path P is SBT1 or SBT2 or SBT3 or an extended peripheral path or a peripheral twin path it will be also called a *candidate path*. Fig. 6 represents examples of candidate paths with corresponding hexagons colored gray.

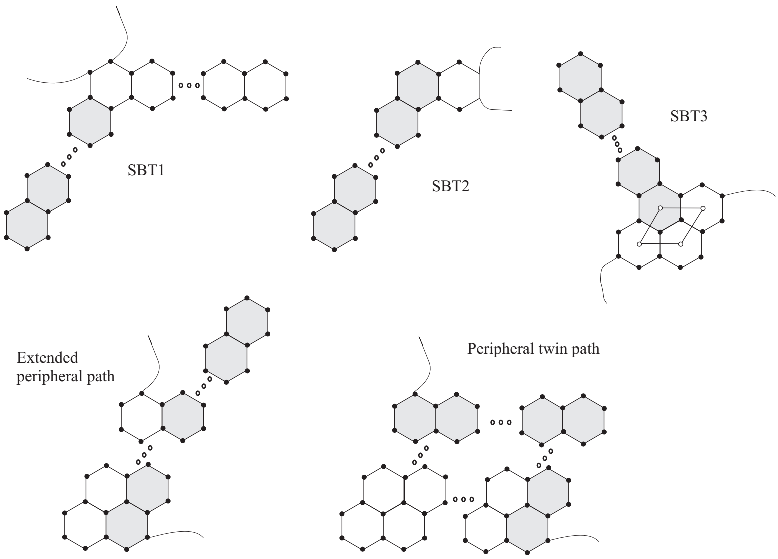

Figure 6: Candidate paths.

If $P = u_1, u_2, \ldots, u_k$ is a candidate path of G but not a peripheral twin path, then we shall always choose the notation such that $d_{I(G)}(u_1) = 1$.

A peripheral path $u_1, \ldots, u_i, v, v_1, \ldots, v_j$ is called to be *reducible* if v_j is a reducible hexagon. A peripheral twin path P is *reducible* if both peripheral paths of P are reducible. If $u_1, \ldots, u_i, v, v_1, \ldots, v_j$ is a reducible extended peripheral path, then $u_1, \ldots, u_i, v_j, v_{j-1}, \ldots, v_1, v$ is called a *sequence of reducible hexagons induced by* P. If $w_1, w_2, \ldots, w_k$ is a sequence of reducible hexagons induced by P, then we set $G_i := G - w_1 - \ldots - w_i$ for $i = 0, 1, \ldots, k$. If G is elementary, then it is easy to see that G_i is also elementary. Analogously, if the paths $u_1, \ldots, u_i, v$ and $v_1, \ldots, v_j, v$ compose a peripheral twin path with a critical point v, then $u_1, \ldots, u_i, v, v_j, v_{j-1}, \ldots, v_1$ is a sequence of reducible hexagons induced by P.

It is not difficult to see that if $P = v_1, \ldots, v_j$ is a SBT1 or a SBT2 or a SBT3, then $v_1, \ldots, v_j$ is always a sequence of reducible hexagons. Therefore we define: a candidate path P is *reducible* if P is a SBT1 or a SBT2 or a SBT3 or a reducible extended peripheral path or a reducible peripheral twin path.

Proposition 8. *If H is a pericondensed component of an elementary benzenoid graph G without nice coronenes, then $I(H)$ admits at least two reducible peripheral twin paths.*

Proof. If H is convex, then H is a parallelogram and we are done.

If H is not convex, let S denote its 4-tiling. The proposition clearly holds if $I_S(H)$ admits exactly two 4-cycles. Suppose then that H is a pericondensed graph with the least number of hexagons such that H does not admit two peripheral twin paths. Note that H admits at least two $\frac{2\pi}{3}$ turns by Proposition 7. Moreover, since H does not admit two reducible twin paths, it admits at least one critical point v that does not induce a reducible twin path. If $v, v_1, \ldots, v_j$ is a non-reducible peripheral path induced by v, then v_j is not removable by Proposition 6 and we have $d_{I_S(H)}(v_j) \geq 4$. Moreover, v_j is peripheral and we get $d_{I_S(H)}(v_j) = 4$ (see Fig. 5c).

Let $P_v = v, v_1, \ldots, v_j, u_1, \ldots, u_k$ denote the maximal straight path in $I_S(H)$. Note that $d_{I_S(H)}(u_k) = 3$ and since u_k by Proposition 4 cannot be internal, it admits a $-\frac{\pi}{3}$ turn. Since v_1 and u_k are peripheral and H is not a coronoid, the removal of vertices of P_v disconnects H. Moreover, P_v partition H into two subgraphs, say H_1 and H_2, such that the hexagons of $v_j, u_1, \ldots, u_k$ form the intersection of H_1 and H_2. Note that both H_1 and H_2 are elementary. By assumption, H admits at most one reducible twin path P and let P belong to H_2. Then H_1 admits at most one reducible peripheral twin paths (P_v in H_1 yields at most one new $\frac{2\pi}{3}$ turn). Since H_1 possesses less hexagons then H, we obtain a contradiction. ■

Lemma 2. *Let G be a benzenoid graph without nice coronenes. If P is a candidate path of G, then a 1-factor of G admits at most one pairwise disjoint resonant hexagon of P.*

Proof. Assume first that P is not a peripheral twin path. We will show that a perfect matching M of H admits in P at most one edge perpendicular to the straight line defined by P. Suppose that M possesses two such edges, say e and e'. We now choose x and y to be the end-vertices of e and e', respectively, such that both belong to ∂G and the distance between x and y in ∂G is minimal. Let L_e denote the shortest path between x and y (x and y excluded) in ∂G. Since x and y are of the same color, L_e is obviously a path with an odd number of vertices and thus cannot be M-alternating. Edges of L_e are peripheral, hence M cannot exist. From the obtained contradiction it follows that a perfect matching of G admits at most one pairwise disjoint resonant hexagon of P and the case is settled.

We assume now that P is a peripheral twin path with the critical point v. Note that the hexagon v contains two edges, say e_1 and e_2, that are not adjacent to any other hexagon of G. It follows that a perfect matching M has to contain exactly one of e_1 and e_2. Suppose w.l.o.g. that M contains e_1. Note that P is composed of two maximal straight paths; one of them, say P_1, is perpendicular to e_1 and the other, say P_2, is perpendicular to e_2. Suppose now that M admits a resonant hexagon $h \neq v$ of P_1. Then M has to admit an edge $e \neq e_1$ perpendicular to P_1 and analogously as above we obtain a contradiction. Since M admits at most one resonant hexagon in P_2, the proof is complete. ■

Let h be a removable hexagon that admits a $\frac{\pi}{3}$ turn in an elementary benzenoid graph G and let S be a 4-tiling of G. The the *internal cut* $P_h = h, u_1, \ldots, u_k$ corresponding to h is the maximal straight path in $I(G)$ such that $hu_1 \in S$ and every edge u_iu_{i+1}, $i = 1, \ldots, k-1$, lies on the same line as hu_1.

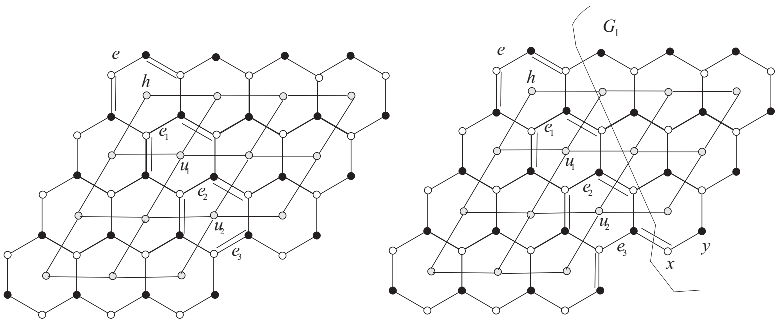

Figure 7: Illustration to the proof of Lemma 3

It was shown in [8] that if an edge e of a benzenoid graph G with a perfect matching M is on a M-resonant cycle, then e is on M'-resonant cycle for every perfect matching M' of G. Moreover, Theorem 3 implies that a benzenoid graph G is elementary if and only if every edge of G is on a M-resonant cycle for a perfect matching M of G. The above observations give the following

Corollary 2. *If e is an edge of an elementary benzenoid graph G with a perfect matching M, then e is on a M-resonant cycle.*

Lemma 3. *If h is a reducible hexagon of an elementary benzenoid graph without nice coronenes G such that the degree of h in $I(G)$ is either one or three, then $Cl(G) \leq Cl(G-h)+1$. Moreover, if $Cl(G) = Cl(G-h)+1$, then G admits a Clar formula R such that $h \in R$.*

Proof. Let h is of degree one in $I(G)$ and e the edge in the intersection of G and $G-h$. Let M denote a perfect matching of G with $Cl(G)$ pairwise disjoint resonant hexagons. Note that M admits either one or two edges of h with end-vertices of degree two. Let M' denote the restriction of M to $G-h$. If M possesses one edge of h with end-vertices of degree two, then set $M' := M \cup \{e\}$. It is straightforward to see that M' is a perfect matching of $G-h$. Hence, M' admits at least $Cl(G)-1$ pairwise disjoint resonant hexagons in $G-h$ and we have $Cl(G) \leq Cl(G-h)+1$. Since the number of pairwise disjoint resonant hexagons of M cannot be equal to $Cl(G-h)+1$ if h is not M-resonant, this case is settled.

Let h is of degree three in $I(G)$ and e the edge of h with end-vertices of degree two. Let M denote a perfect matching of G with $Cl(G)$ pairwise disjoint resonant hexagons. Note that M either admits e or not. If $e \in M$, then let M' denote the restriction of M to $G-h$. It is straightforward to see that M' is a perfect matching of $G-h$. Hence, M' admits at least $Cl(G)-1$ pairwise disjoint resonant hexagons in $G-h$ and we have $Cl(G) \leq Cl(G-h)+1$.

If $e \notin M$, then observe the internal cut $P_h = h, u_1, \ldots, u_k$ corresponding to h. Let e_1 denote the edge in the intersection between h and u_1, let e_i denote the edge in the intersection between u_{i-1} and u_i, $i = 2, \ldots, k$ and let e_{k+1} denote the peripheral edge of u_k. If $e_i \in M$, $i = 1, \ldots, k$, then h_{i-1} is M-resonant (see the left hand side of Fig. 7). Moreover, $M' := M \oplus u_{i-1} \ldots \oplus u_1 \oplus h$ is a perfect matching of G such that $e \in M$ and we obtain the above case.

Suppose then $e_i \notin M$ for every $i = 1, \ldots, k$ (see the right hand side of Fig. 7). By Corollary 2 the edge e_{k+1} has to be on a M-resonant cycle. Let us denote this cycle by C. Note that the edges of u_k adjacent to e_{k+1} are not in M and therefore cannot belong to C. If follows that two peripheral edges adjacent to e_{k+1} belong to C. Let denote one of them e' and let x denote the end-vertex of e' that does not belong to u_k. Note that x is of degree two, hence, the peripheral edge xy has to belong to C. Note also that by removing vertices of P_h we obtain two connected components of G, say G_1 and G_2. Suppose $x \in V(G_1)$. We can see that vertices of P_h are all covered by M. It follows that C admits an M-alternating path that begins in y and ends in a vertex of G_1, say z, adjacent to a vertex of P_h. But since y and z are both of the same color, this path is of even length and we obtain a contradiction. It follows that M cannot be a perfect matching of G. This contradiction completes the proof. ■

Let G denote an elementary benzenoid graph and P a candidate path in G. Let also $\mathcal{H}(G)$ and $\mathcal{H}(P)$ stand for the set of hexagons of G and P, respectively. We denote by $G - P$ the subgraph of G induced by the hexagons of $\mathcal{H}(G) \setminus \mathcal{H}(P)$.

Lemma 4. *If P is a reducible candidate path of an elementary benzenoid graph without nice coronenes G, then $Cl(G) \leq Cl(G - P) + 1$.*

Proof. Let $u_1, u_2, \ldots, u_k$ denote a sequence of reducible hexagons induced by P. We also set $G_i := G - u_1 - \ldots - u_i$ for $i = 0, 1, \ldots, k$. We claim that $Cl(G_i) \leq Cl(G-P)+1$. Note that $G_k = G-P$. Hence, from Lemma 3 it follows that $Cl(G_{k-1}) \leq Cl(G-P)+1$. Suppose to the contrary that $Cl(G_t) > Cl(G-P)+1$ for some $t < k-1$ and $Cl(G_i) \leq Cl(G-P)+1$ for every $i > t$. From Lemma 3 then it follows that $Cl(G_t) = Cl(G_{t+1}) + 1$. Moreover, G_t admits a perfect matching M which induces a Clar formula R such that $u_{t+1} \in R$. If u_{t+1} is of degree one (resp. three) in G_t, then we may assume w.l.o.g. that the edge in the intersection of u_{t+1} and u_{t+2} (resp. the edge with end-vertices of degree two) belongs to M.

If P is a SBT1, then u_{t+2} is also M-resonant (note that $t \leq k - 2$). Let M' denote the restriction of M to G_{t+1}. If $t = k - 2$, then the hexagon of $G - P$ adjacent to u_k, cannot be M resonant. Analogously, if $t < k - 2$, then u_{t+3} cannot be M-resonant. It follows that M' admits $Cl(G_t)$ pairwise disjoint resonant hexagons in G_{t+1} and we obtain a contradiction.

If P is a SBT2, then suppose first that $t = k - 2$. Let M' denote the restriction of M to $G - P$. Since M' admits $Cl(G) - 1$ pairwise disjoint resonant hexagons in $G - P$, we obtain a contradiction. If $t < k-2$, then let M' denote the restriction of M to G_{t+1}. Note that u_{t+2} is also M-resonant and u_{t+3} cannot be M-resonant. It follows that M' admits $Cl(G_t)$ pairwise disjoint resonant hexagons in G_{t+1} and we obtain a contradiction.

If P is a SBT3, then suppose first that $t < k - 2$. Let M' denote the restriction of M to G_{t+1}. We can see that u_{t+2} is also M-resonant and u_{t+3} cannot be M-resonant. It follows that M' admits $Cl(G_t)$ pairwise disjoint resonant hexagons in G_{t+1} and we obtain a contradiction. Let the $t = k-2$ and let M' denote the restriction of M to $G-P$. Note that u_k and u_{k-1} admit together exactly one disjoint resonant set in G_t. It follows that $Cl(G_t) \leq Cl(G-P)+1$ and since we obtain a contradiction this case is settled.

If P is an extended peripheral path, then assume first that u_{t+1} belongs to a beam of G. We can see that the hexagons $u_{t+1}, \ldots, u_k$ form a SBT2 in G_t. Since we can obtain a contradiction analogously as above, this case is settled. Let then u_{t+1} be a hexagon that belongs to a pericondensed component of G and let $u_\ell \neq u_k$ be the hexagon of a pericondensed component with the largest index. Note that $Cl(G_\ell) \leq Cl(G-P)+1$. Suppose that $Cl(G_i) \leq Cl(G-P)+1$ for every $\ell \leq i < t$. If $t > \ell+1$, then u_{t+2} is also M-resonant and u_i cannot be M resonant for $t+2 < i \leq k$ by Lemma 2. If $t = \ell+1$, then u_ℓ is also M-resonant and u_i cannot be M resonant for $t+2 < i < k$. A hexagon of $G-P$ adjacent to a hexagon of $u_{t+1}, \ldots, u_k$ cannot be M-resonant since a boundary of the subgraph induced by the hexagons $u_{t+1}, \ldots, u_k$ is M-resonant as depicted in the example in the left-hand side of Fig. 8. It follows that u_{t+2} is not adjacent to any M-resonant hexagon except to u_{t+1}. Let M' denote the restriction of M to G_{t+1}. From the discussion above it follows that M' is a perfect matching of G_{t+1} with $Cl(G_t)$ pairwise disjoint resonant hexagons and we are done.

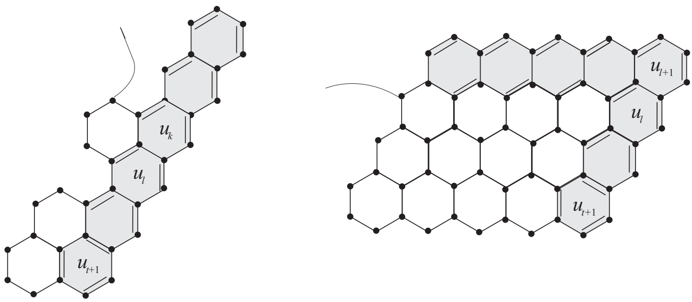

Figure 8: Illustration to the proof of Lemma 4

If P is a peripheral twin path, then note that P is composed of two peripheral paths, say P_1 and P_2. Let $P_1 = u_1, \ldots, u_{\ell+1}$ and $P_2 = u_{\ell+1}, \ldots, u_{k-1}, u_k$, such that $u_{\ell+1}$ is the critical point of P. Assume first that u_{t+1} belongs to P_2. We can see that the hexagons $u_{t+1}, \ldots, u_k$ form an extended peripheral path in G_t. Since we can obtain a contradiction analogously as above, this case is settled. Let then u_{t+1} be a hexagon that belongs to P_1. Note that $Cl(G_\ell) \leq Cl(G-P)+1$. Suppose now that $Cl(G_i) \leq Cl(G-P)+1$ for every $\ell \leq i < t$. We can see that u_{t+2} is also M-resonant. Moreover, u_i cannot be M resonant for $t+2 < i \leq k$ by Lemma 2. A hexagon of $G - P$ adjacent to a hexagon of $u_{t+1}, \ldots, u_k$ cannot be M-resonant as depicted in the example in the right-hand side of Fig. 8. It follows that u_{t+2} is not adjacent to any M-resonant hexagon except to u_{t+1}. Let M' denote the restriction of M to G_{t+1}. From the discussion above it follows that M' is a perfect matching of G_{t+1} with $Cl(G_t)$ pairwise disjoint resonant hexagons and we obtain a contradiction. This assertion completes the proof. ■

For the convenience, we will assume that G is composed of a single SBT1, if G is a linear hexagonal chain.

Theorem 4. *If G is an elementary benzenoid graph without nice coronenes, then there exists a reducible candidate path P of G such that the following hold:*

(i) $G - P$ is an elementary benzenoid graph without nice coronenes,

(ii) $Cl(G - P) = Cl(G) - 1$.

Proof. If G is a linear hexagonal chain, then the proof is trivial. Suppose then that G is not a linear hexagonal chain.

We will distinguish the following two cases.

A. G admits P which is a SBT1 or a SBT2 or a SBT3. Let $P = u_1, u_2, \ldots, u_k$ such that u_1 is the vertex of degree one.

(i) It is easy to see that the sequence of hexagons $u_1, u_2, \ldots, u_k$ is reducible.

(ii) Because of Lemma 4 we only have to show $Cl(G - P) \leq Cl(G) - 1$.

If P is a SBT1, then let $v \neq u_{k-1}$ denote the hexagon adjacent to u_k and e the edge in the intersection of u_k and v. Let also P' denote the other SBT1 which intersects in v and let v' denote the hexagon of P' adjacent to v. Suppose M' is a perfect matching of $G - P$ with $Cl(G - P)$ pairwise disjoint resonant hexagons and R a set of resonant hexagons of G of the same cardinality induced by M'. If R contains v, then P' by Lemma 2 cannot admit any other resonant hexagon in R. It follows that either M' or $M' \oplus v$ admits a set of resonant hexagons $R' := R \setminus \{v\} \cup \{v'\}$. In the latter case we set $M' := M' \oplus v$. Note that R' is the set of cardinality $Cl(G - P)$. Let M_e be the perfect matching of P such that $e \in M_e$ and u_k is M_e-resonant. Hence, $M' \cup M_e$ is a perfect matching of G with $Cl(G - P) + 1$ pairwise disjoint resonant hexagons. If R does not contain v, we can find analogously a perfect matching of G with $Cl(G - P) + 1$ pairwise disjoint resonant hexagons. It follows that $Cl(G - P) \leq Cl(G) - 1$.

If $P = u_1, u_2, \ldots, u_k$ is a SBT2, note that $k \geq 2$. Let $v \neq u_{k-1}$ denote the hexagon adjacent to u_k and e the edge in the intersection of u_k and v. If M' is a perfect matching of $G - P$ with $Cl(G - P)$ pairwise disjoint resonant hexagons, then we can find a perfect matching M_e of P which contains the edge e such that a hexagon u_{k-1} is resonant. Then $M := M' \cup M_e \setminus \{e\}$ is a perfect matching of G with $Cl(G - P) + 1$ pairwise disjoint resonant hexagons. It follows that $Cl(G) \geq Cl(G - P) + 1$ and $Cl(G - P) \leq Cl(G) - 1$.

If P is a SBT3, then let e denote the edge in the intersection of u_k and u_{k-1}. If M' is a perfect matching of $G - P$ with $Cl(G - P)$ pairwise disjoint resonant hexagons and M_P a perfect matching of the graph induced by $u_1, u_2, \ldots, u_{k-1}$ such that u_1 is M_P-resonant, then $M' \cup M_P$ is a perfect matching of G with $Cl(G - P) + 1$ pairwise disjoint resonant hexagons. It follows that $Cl(G) \geq Cl(G - P) + 1$ and $Cl(G - P) \leq Cl(G) - 1$.

B. G does not possess a SBT1 or SBT2 or SBT3.

(i) Proposition 8 says that every pericondensed component of G admits at least two reducible twin paths. If G possesses exactly one pericondensed component, then, since G does not possess a SBT1 or SBT2 or SBT3, it clearly admits a reducible extended peripheral path or a reducible twin path P. Suppose then that G consists of more then one pericondensed component. Since G admits no finite face besides hexagons, it has to admit at least two pericondensed components, say H_1 and H_2, with exactly one link. Let H denote the subgraph of G composed of H_1 and beams adjacent to H_1. Since G does not possess a SBT1 or SBT2 or SBT3 and since H_1 has exactly one link, it follows that H (and therefore G) admits at least one reducible extended peripheral path or a reducible twin path P. From Corollary 1 it follows that $G - P$ is an elementary benzenoid graph without nice coronenes and this part is settled.

(ii) We only have to show $Cl(G - P) \leq Cl(G) - 1$.

Assume first that $P = u_1, \ldots, u_k, v, v_1, \ldots, v_j$ is an extended peripheral path, where v is a peripheral vertex of $I(G)$ which admits a $\frac{2\pi}{3}$ turn in a pericondensed component of G and u_1 is of degree one. Let L_v denote the subgraph of G induced by the vertices that do not belong to $G - P$. Note that L_v is path of odd length. Suppose M' is a perfect matching of $G - P$ with $Cl(G - P)$ pairwise disjoint resonant hexagons and R a set of resonant hexagons of G of the same cardinality induced by M'. Let M_v be a perfect matching of L_v such that u_1 is M_v resonant and set $M := M' \cup M_v$. It is easy to see now that M is a perfect matching of G, Moreover, M possesses $Cl(G - P) + 1$ pairwise disjoint resonance hexagons, since $R \cup \{u_1\}$ is resonance set. It follows that $C(G) \geq Cl(G - P) + 1$.

Assume now that $P = u_1, \ldots, u_i, v, v_1, \ldots, v_j$ is a peripheral twin path, with a critical point v, while u_1 and v_j are the end-vertices of P. Let L_v denote the subgraph of G induced by the vertices that do not belong to $G-P$. Note that L_v is composed of a single hexagon v to which two paths with even numbers of vertices are attached. Suppose M' is a perfect matching of $G-P$ with $Cl(G-P)$ pairwise disjoint resonant hexagons and R a set of resonant hexagons of G of the same cardinality induced by M'. From the discussion above it follows that L_v admits a perfect matching, say M_v, such that v is M_v-resonant. Let $M := M' \cup M_v$. It is easy to see now that M is a perfect matching of G, Moreover, M possesses $Cl(G-P)+1$ pairwise disjoint resonance hexagons, since $R \cup \{v\}$ is its resonance set. It follows that $C(G) \geq Cl(G-P)+1$. This assertion completes the proof. ■

From Theorem 4 and from its proof follows the next

Corollary 3. *If G is an elementary pericondensed benzenoid graph without nice coronenes, then G admits a reducible candidate path $P = u_1, \ldots, u_k$ and a Clar formula R such that*

$u_k \in R$ if P is a SBT1;

$u_{k-1} \in R$ if P is a SBT2 or SBT3;

$u_1 \in R$ if P is an extended peripheral path;

$v \in R$ if P is a peripheral twin path with a critical point v.

3 Algorithm

If P is a straight path in $I(G)$ and h a hexagon adjacent to P, then let $P+h$ denotes the path composed as the union of hexagons of P and h. Analogously, if h is an end-vertex of P, then $P-h$ denotes the path composed of hexagons of P but without h.

If G is an elementary pericondensed benzenoid graph without nice coronenes, then $\mathcal{P}(G)$ denotes the set of reducible candidate paths of G.

Claim 1. *Let G be an elementary pericondensed benzenoid graph without nice coronenes. If $P, Q \in \mathcal{P}(G)$, then $Q \in \mathcal{P}(G-P)$ unless*

(i) P and Q intersect in a hexagon h and then $Q-h \in \mathcal{P}(G-P)$,

(ii) P and Q are both SBT1 and adjacent to a common hexagon of degree three h and then $Q+h \in \mathcal{P}(G-P)$.

Proof. If P is a SBT1 in G, then there exists the path Q which is also a SBT1 in G such that P and Q are adjacent to a common hexagon of degree three h. We can easily see that $Q + h$ is a SBT2 in $G - P$.

If P is a SBT2 or SBT3, then, since P cannot intersect with Q, it follows that $Q \in \mathcal{P}(G - P)$.

Suppose finally that P (resp. Q) is either an extended peripheral path or a peripheral twin path. We can see that P and Q intersect in h only if h admits a $\frac{\pi}{3}$ or $-\frac{\pi}{3}$ turn. If h' is a hexagon of Q adjacent to h, then h' is reducible hexagon in $G - P$. It follows that $Q - h$ is reducible candidate path of $G - P$. This assertion concludes the proof. ∎

Claim 2. *Let G be an elementary pericondensed benzenoid graph without nice coronenes and $P \in \mathcal{P}(G)$. If $P' \in \mathcal{P}(G - P)$ such that $P' \notin \mathcal{P}(G)$ and P is not obtained as suggested in Claim 1, then P is either a SBT2 or a SBT3 or an extended peripheral path or a peripheral twin path.*

Proof. Let S denote a 4-tiling of G. If P is a SBT1, then the removal of P from G affects only the path Q which is also a SBT1 in G such that P and Q are adjacent to a common hexagon of degree three h as suggested in Claim 1 (ii).

If P is a SBT2, then an end-vertex of P is a adjacent to a hexagon h which is of degree one in $G - P$ and therefore it can induce a path in $\mathcal{P}(G - P)$.

If P is a SBT3, then the end-vertex of P is a adjacent to two hexagons, say h and h', in $I_S(G)$. Moreover, h (resp. h') can be reducible in $G - P$ or it belongs to a beam of $G - P$ and therefore it can induce a path in $\mathcal{P}(G - P)$.

If P is an extended peripheral path, let h' denote the hexagon of P of degree three in $I(G)$ and h the hexagon adjacent to the hexagon h' in $I_S(G - P)$. Note that h can be reducible in $G - P$ and therefore it can induce a path in $\mathcal{P}(G - P)$.

If P is a peripheral twin path, an end-vertex of P is adjacent to the hexagon h in $I_S(G - P)$. Again, h can be reducible in $G - P$ and therefore it can induce a path in $\mathcal{P}(G - P)$.

Since we settled all cases, the assertion follows. ∎

A hexagon h from the proof of Claim 2 is called a *candidate hexagon*.

Theorem 4 is the basis for the next algorithm.

Linear Clar

input - an elementary benzenoid graph G.
output - a Clar formula R of G.

1. $I_G :=$ the inner dual of G.
2. $S :=$ the 4-tilling of M.
3. $\mathcal{P} := \{P;\ P = u_1, \ldots, u_k$ is a reducible candidate path of G $\}$.
4. **repeat**
   (a) Choose P be a path of $\mathcal{P}$.
   (b) **case** P is
   a SBT1: $R := R \cup \{u_k\}$.
   a SBT2 or SBT3: $R := R \cup \{u_{k-1}\}$.
   an extended peripheral path: $R := R \cup \{u_1\}$.
   a peripheral twin path: $R := R \cup \{$the critical point of $P\}$.
   end case
   (c) $\mathcal{P} := \mathcal{P} \setminus \{P\}$.
   (d) update $\mathcal{P}$ as follows:
   i. **if** P and $P' \in \mathcal{P}$ intersect in hexagon h, **then** remove h from P'.
   ii. **if** P is a SBT1 such that P' shares the hexagon h with P, **then** augment P' with h.
   iii. **if** P is not a SBT1, **then** insert in $\mathcal{P}$ new reducible candidate paths induced by removal of P from G.
   (e) Remove hexagons of P from G.
   until $\mathcal{P}$ is an empty set.

Theorem 5. *Algorithm Linear Clar finds a Clar formula of an elementary benzenoid graph G and can be implemented to run in $O(n)$ time.*

Proof. The correctness of the algorithm follows from Theorem 4 and Corollary 3. Starting from G, the algorithm at each execution of the loop choose a path P from the set of reducible candidate paths $\mathcal{P}$. A hexagon of P is inserted in the set of resonance hexagons R with respect to Corollary 3. The set of reducible candidate paths $\mathcal{P}$ is then updated in Step 4d as sugested in Claims 1 and 2. Finally, the hexagons of P are removed from G and the resulting graph is elementary. The body of the loop is executed until $\mathcal{P}$ is empty.

Concerning the time complexity of the algorithm, note that a vertex of G and $I(G)$ possesses at most three and six adjacent vertices, respectively. Thus, the complexities of basic operations: deleting an edge or a vertex, deleting all edges incident with a vertex etc., are constant notwithstanding a representation of G and $I(G)$. It is clear that the inner dual of G can be computed in linear time. It is showed in [13] that the 4-tilling of G can be found within the same time bound. In order to find the set of reducible candidate paths $\mathcal{P}$, the algorithm checks whether a hexagon of degree one or a hexagon which induces a $\frac{2\pi}{3}$ turn (a hexagon of degree three with adjacent neighboring hexagons) admits a reducible candidate path. Since a hexagon h of G is a crossing of at most three peripheral paths, h is checked at most three times during this step which therefore requires linear time.

In order to achieve a desired time bound of the loop, for every hexagon h of G we make a label which shows to which candidate path (if any) h belongs. Note that h can be in at most two candidate paths.

We are left to show that the loop is executed in linear time. Since we choose an arbitrary path of $\mathcal{P}$, Steps 4a, 4b, 4c, and 4d can be implemented to run in time linear in the number of hexagons of P. Finally, $\mathcal{P}$ is updated in Step 4d as illustrated in the proof of Claims 1 and 2. We analyze the complexity of this step below.

If a hexagon h at an end of P can belong to some other path $P' \in \mathcal{P}$, then h is removed from P'. Since we know to which candidate paths h belongs and since h is always an end-vertex of a candidate path, we can compute this step in constant time.

If P is a SBT1, then we first find a hexagon h adjacent to an end-vertex of P. Then we find the hexagon adjacent to h in $G - P$ which is also the hexagon of $P' \in \mathcal{P}$. Finally, P' is augmented with h. Again we can compute this step in constant time.

If P is not a SBT1, then the procedure tries to find new reducible candidate paths in Step 4d (iii). We will show that the notal number of hexagons checked in all runs of this step is bounded with $O(n)$, i.e. we will show that the number of visits to a hexagon of G is constant.

As suggested in the proof of Claim 2, the algorithm first finds a candidate hexagon h which can induce a new path in $\mathcal{P}(G - P)$. A candidate hexagon is adjacent to an end-vertex of P and can be therefore found in constant time.

The algorithm then computes in a current graph the maximal peripheral straight path induced by a candidate hexagon h. If the last hexagon, say v, of this path admits a $\frac{2\pi}{3}$ turn, then the algorithm also computes the other maximal peripheral straight path which includes v (in order to find a reducible twin path). Let $P' = h, u_1, \ldots, u_k$ denote the sequence of hexagons checked in this procedure. We will show that a hexagon of P' is checked at most six times in all runs of the loop.

If P' is a reducible candidate path, then every hexagon of P' is checked exactly once and we are done.

Otherwise, note that a hexagon of P' does not admit a turn in a current graph. A hexagon u_i of P' can become a candidate hexagon in some later execution of the loop when hexagons $u_k, u_{k-1}, \ldots, u_{i+1}$ are already removed from a current graph. If this is the case, then $u_i, u_{i-1}, \ldots, u_1, h$ is a reducible peripheral path, since h is reducible hexagon. It follows that P' is traversed at most twice in all runs of the loop. Since a hexagon of G is a crossing of at most three peripheral paths, a hexagon of G can be checked at most six times. This observation yields the desired running time of the loop. ■

We conclude the paper with the running of Linear Clar given input the graph from Fig. 2. The situation is depicted in Fig. 9. We can see that the reducible candidate paths $P_1, P_2, \ldots, P_8$ are computed and removed from the graph in consecutive executions of the loop. Note also that P_3 is augmented with the hexagon adjacent to P_2 and P_3. Before a candidate path is removed, a hexagon that belong to the computed Clar formula is chosen (marked with a circle in the figure).

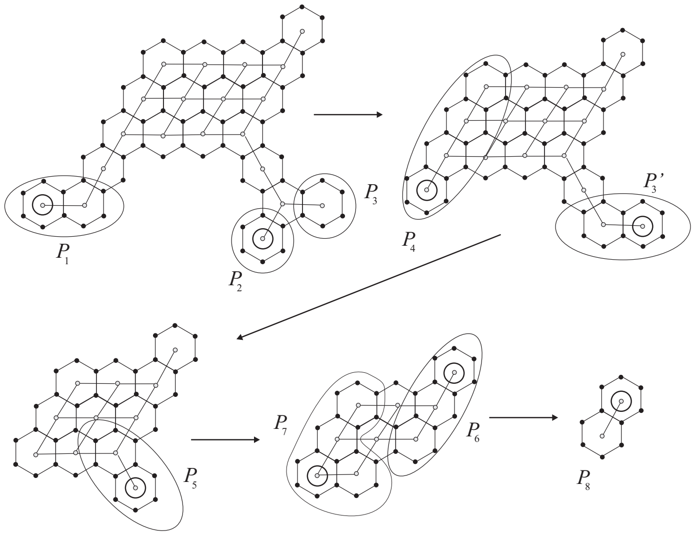

Figure 9: Running of Linear Clar for the graph depicted in Fig. 2.

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