MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **69** (2013) 733-754

ISSN 0340 - 6253

On the Anti-Kekulé Number of a Hexagonal System*

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(Received February 22, 2012)

Abstract

A hexagonal system is a connected plane graph without cut vertices in which each interior face is a regular hexagon. Let H be a hexagonal system. An anti-Kekulé set of H is a set S of edges of H such that $H - S$ is a connected graph that has no Kekulé structures. The minimum of cardinalities of anti-Kekulé sets of H is called the anti-Kekulé number of H, denoted as $ak(H)$. An anti-Kekulé set S of H is called a smallest anti-Kekulé set of H if the cardinality of S equals $ak(H)$. It is obvious that a single hexagon has no anti-Kekulé sets. In this paper, we show that for a hexagonal system H with more than one hexagon, $ak(H) = 0$ if and only if H has no Kekulé structures, $ak(H) = 1$ if and only if H has a fixed double edge, and $ak(H)$ is either 2 or 3 for the other cases. Further by applying perfect path systems we give a characterization whether $ak(H) = 2$ or 3, and present an $\mathrm{O}(n^2)$ algorithm for finding a smallest anti-Kekulé set in a normal hexagonal system, where n is the number of its vertices.

1 Introduction

The anti-Kekulé number was introduced by Vukičević and Trinajstić [17]. In [16], Vukičević proved that the anti-Kekulé number of buckminsterfullerene C_{60} is 4. Kutnar et al obtained that the anti-Kekulé number of a leapfrog fullerene is either 3 or 4 [11]. Afterwards, Yang et al. [20] demonstrated that the anti-Kekulé number of any fullerene

*This work is supported by NSFC (grant no. 10831001).
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graph is 4. In [17, 18], Vukičević and Trinajstić showed that the anti-Kekulé number of benzenoid parallelograms is 2 and the anti-Kekulé number of cata-condensed hexagonal systems is either 2 or 3. Veljan and Vukičević [15] obtained that the anti-Kekulé numbers of the infinite triangular, rectangular and hexagonal grids are 9, 6 and 4 respectively. There is some other study of anti-Kekulé number in [1, 23]. Nevertheless, there are few results about the anti-Kekulé number of any hexagonal system. In this paper, we intend to settle the problem of determining the anti-Kekulé number of any hexagonal system.

For the terms and notations used, but not defined here, we refer the reader to [12, 19]. For a graph G, a *perfect matching* (or *Kekulé structure*) of G is a set of disjoint edges which covers all of its vertices. An *anti-Kekulé set* of G is an edge set S such that $G-S$ is connected and has no Kekulé structures. A smallest anti-Kekulé set of G is an anti-Kekulé set of G with the smallest cardinality, which is called the *anti-Kekulé number* of G and denoted by $ak(G)$.

Let G be a graph with a perfect matching. An edge of G is a *fixed double* (*single*) edge if it belongs to all (none) of the perfect matchings of G. Both fixed double edges and fixed single edges are called *fixed edges*. A bipartite graph with a perfect matching is called *normal* (or *elementary*) if it is connected and has no fixed edges. A plane bipartite graph with a perfect matching is called *weakly elementary*, if for any nice cycle C of G, the edges that are incident with the vertices of C and lie in the interior of C are not fixed single edges. The components of the subgraph of G formed by all non-fixed edges are called the *normal components* of G.

Let G be a 2-connected graph. If every interior face of each normal component of G is a face of G, then the normal component is called a *normal block* of G. For a path $P = v_1v_2 \ldots v_n$ of G, let $d(v_i)$ be the degree of v_i in G ($i = 1, \ldots, n$). Then we say G has a $(d(v_1), d(v_2), \ldots, d(v_n))$ path P.

A *hexagonal* (*benzenoid*) *system* H is a connected plane graph without cut vertices in which each interior face is a regular hexagon of side length one. The carbon-skeleton of a benzenoid hydrocarbon is a Kekuléan hexagonal system, i.e. it has a Kekulé structure [2, 4, 5]. So chemists and graph theorists are both interested in this kind of graphs. A hexagonal system is said to be *cata-condensed* if no three of its hexagons share a common vertex; otherwise, it is *pericondensed*.

It is obvious that $ak(H) = 0$ if and only if H is a non-Kekuléan hexagonal system.

For a Kekuléan hexagonal system H, since a single hexagon has no anti-Kekulé sets, we always assume that H has at least two hexagons in the following. If H has a fixed double edge, then after deleting the fixed double edge from H, the remaining subgraph is still connected and has no Kekulé structures, which implies that $ak(H) = 1$. Conversely, if $ak(H) = 1$, then the edge which forms an anti-Kekulé set belongs to all of the perfect matchings of H and is thus a fixed double edge of H. Hence $ak(H) = 1$ if and only if H has a fixed double edge. For hexagonal systems with fixed single edges but no fixed double edges, the situation is somewhat complicated. But since the fixed single edges are not contained in any smallest anti-Kekulé set of H, we can simplify the problem by deleting all the fixed single edges. For the components of the remaining subgraph, we have the following theorem.

Theorem 1.1. *[10] Let H be a hexagonal system. If H has fixed edges, then it has at least two normal components.*

The following theorem points out that the normal components cannot all consist of only one hexagon.

Theorem 1.2. *[14] Let G be a 2-connected and weakly elementary plane bipartite graph. Assume that G has more than one cycle and all vertices of degree 2 lie on the boundary of G. If G has m ($m \geq 1$) distinct cycles as normal blocks, then G has $m+2$ normal blocks.*

Every hexagonal system with a perfect matching is weakly elementary [22]. Hence by Theorems 1.1 and 1.2, if H has fixed single edges but no fixed double edges, then H has at least two normal components each of which contains more than one hexagon. Hence $ak(H)$ is equal to the smallest number of the anti-Kekulé numbers of all normal components with more than one hexagon. In [7], a linear algorithm for finding all fixed edges of hexagonal systems was given. Consequently, for a Kekuléan hexagonal system H with fixed single edges but no fixed double edges, we change the problem of determining $ak(H)$ into the problem of determining the anti-Kekulé numbers of all normal components with more than one hexagon of H. Therefore, we just need to consider the normal hexagonal system with more than one hexagon.

In Section 2, we prove that the anti-Kekulé number of any normal hexagonal system with more than one hexagon is either 2 or 3. This result together with the above discussions show that a Kekuléan hexagonal system without fixed double edges has anti-Kekulé number 2 or 3. In particular, we show that the anti-Kekulé number of any normal hexagonal system with a (2, 3, 2) path is 2. In Section 3, we will recall a perfect path system which is the main tool for the proof of our main results. Some lemmas relevant to perfect path systems are also presented. In Section 4, we obtain a characterization of a normal hexagonal system whose anti-Kekulé number is 2. Based on the characterization, in Section 5 an $O(n^2)$ algorithm for finding a smallest anti-Kekulé set in a normal hexagonal system is given, where n is the number of its vertices.

2 The anti-Kekulé number of hexagonal systems

To determine whether or not a given hexagonal system H is normal, we have the following theorem.

Theorem 2.1. *[21] Let H be a hexagonal system. Then H is normal if and only if there exists a perfect matching M of H such that the contour of H is an M-alternating cycle.*

An edge of H is *peripheral* if it is on the boundary of the exterior face of H. Otherwise, it is an *inner* edge.

Lemma 2.2. *$S = \{e, f\}$ is an edge-cut of H if and only if e, f are peripheral edges of H and in the same hexagon.*

Proof. If $\{e, f\}$ is an edge-cut of H and one of e and f, say e, is not peripheral, then there are two hexagons h_1 and h_2 such that $h_1 \cap h_2 = \{e\}$. Since at least one of h_1 and h_2, say h_1, does not contain f. Hence $h_1 \subset H - f$, which implies that deleting e from $H - f$ does not increase the number of components of $H - f$. Since $H - \{e, f\}$ has at least two components, $H - f$ has at least two components. Hence f is a cut edge. But H is 2-connected, a contradiction. Hence both of e and f are peripheral. Suppose $e \in h_1$, $f \in h_2$. If $h_1 \neq h_2$, then deleting e from $H - f$ does not increase the number of components of $H - f$. Hence f is a cut edge of H, a contradiction. Then e and f are peripheral edges of H and in the same hexagon.

If e and f are peripheral edges of H and in the same hexagon, then $H - \{e, f\}$ has two components, each of which has at least one vertex. Hence $\{e, f\}$ is an edge-cut of H. ■

For $e \in E(G)$, let $H - e$ be the graph obtained from H by deleting e but not its end vertices. For $X \subset V(H)$, let $\nabla(X)$ denote the set of edges with only one end vertex in X.

Proposition 2.3. *Let H be a normal hexagonal system with more than one hexagon. Then $ak(H)$ is either 2 or 3. Moreover, if H has a (2, 3, 2) path, then $ak(H) = 2$.*

Proof. Since H is a normal hexagonal system, H has no fixed edges. Hence for any $e \in E(H)$, $H - e$ has perfect matchings, which implies that $ak(H) \geq 2$. On the other hand, the degree of any vertex on the boundary of H is either 2 or 3. Consequently, there is an edge, say uv, with $d(u) = 2$, $d(v) = 3$. Let w be another neighbor vertex of v such that uvw is a path on the boundary of H, we have $d(w) \leq 3$. If $d(w) = 2$, then by Lemma 2.2, $H - \nabla(\{u, w\}) + \{uv, vw\}$ is connected. Note that $H - \nabla(\{u, w\}) + \{uv, vw\}$ has no perfect matchings. Hence $ak(H) = 2$. If $d(w) = 3$, then let the neighbor vertex of u be u_1, the neighbor vertices of w be w_1 and w_2. Denote the three hexagons containing uu_1, ww_1 and ww_2 by h_i (i=1, 2, 3, see Fig. 1). Let $H' = H - \{uu_1, ww_1, ww_2\}$. Note that H' has no perfect matchings. If we can show that H' is connected, then the proposition will be established. For any two vertices x, y of $V(H')$, there is a path P connecting x and y in H. If P contains uu_1 (resp. ww_1), then we replace uu_1 (resp. ww_1) by $\partial(h_1) - uu_1$ (resp. $\partial(h_2) - ww_1$). If P contains ww_2, then we replace ww_2 by $\partial(h_2 \cup h_3) - ww_2$. Hence there is a walk connecting x and y in H'. Since every x,y-walk contains an x, y-path, there is an x, y-path in H'. Hence H' is connected. ■

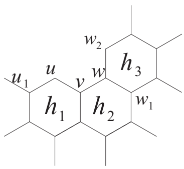


Fig. 1. Illustration for the proof of Proposition 2.3.

For a normal hexagonal system without any (2, 3, 2) path, the two graphs in Fig. 2 indicate that its anti-Kekulé number may be 2 or 3: for the graph G_1, by Theorem 2.1, we can see that it is normal. Color the vertices of G_1 with white and black as shown in Fig. 2. Let Q be the set of the 21 white vertices in the left component of $G_1 - \{e_1, e_2, f_e, f_e^l\}$. Then the neighborhood of Q in $G_1 - \{f_e, f_e^l\}$ consists of only 20 vertices. By Hall's Theorem, $G_1 - \{f_e, f_e^l\}$ has no perfect matchings. Then $\{f_e, f_e^l\}$ is an anti-Kekulé set of G_1. For the graph G_2, in [18], it was proved that the anti-Kekulé number of such a cata-condensed hexagonal system is 3.

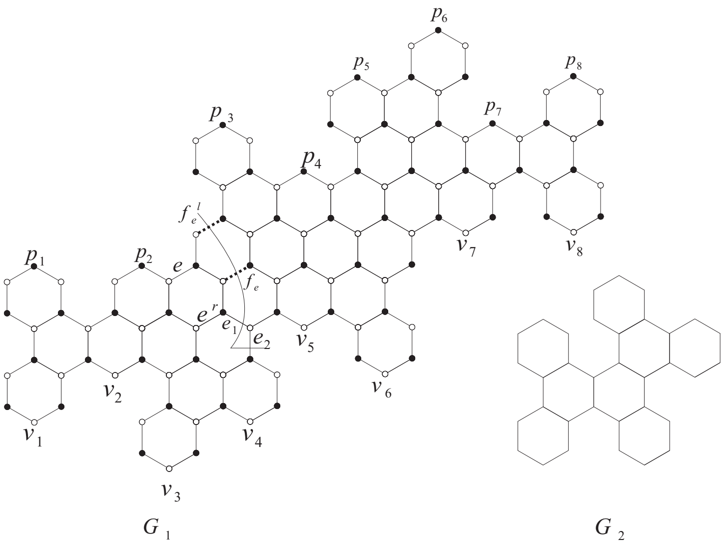


Fig. 2. Two normal hexagonal systems without any (2, 3, 2) path.

Combining the discussions in the introduction and Proposition 2.3, we have the the following corollary.

Corollary 2.4. *The anti-Kekulé number of a Kekuléan hexagonal system without fixed double edges is 2 or 3.*

3 Perfect path systems and some lemmas

Let H be a hexagonal system. A straight line segment C with end points P_1, P_2 is called a cut segment of H if

(a) C is orthogonal to one of the three edge directions ,

(b) each of P_1, P_2 is the center of an edge lying on the contour of H,

(c) the graph obtained from H by deleting all edges intersected by C has exactly two components.

From now on, we always let H be a normal hexagonal system embedded in the plane with some of its edges vertical. For a hexagonal chain of H, the *range* of the chain is defined by the set of all the horizontal cut segments intersecting the chain (see Fig. 3). A *peak* (*valley*) of H is a vertex all of whose neighbors are below (above) it. Thus a peak or a valley has degree 2.

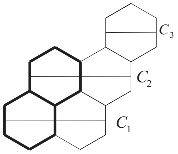


Fig. 3. The range of the hexagonal chain shown in bold is $\{C_1, C_2\}$.

A *monotone path system* of H is a set of disjoint monotonically down paths of H in which each path issues at a peak and ends at a valley. A *perfect path system* of H is a monotone path system which covers all peaks and valleys. In [3, 13], it was formally proved that there is a one-to-one correspondence between perfect path systems and perfect matchings of H. The correspondence is as follows: take all non-vertical edges in and vertical edges not in the paths of a perfect path system and a perfect matching is obtained; on the other hand, for a perfect matching deleting all vertical double edges together with their end vertices from H, a perfect path system is found.

In [6, 13], it was proved that if H has a perfect path system, then the induced matching between peaks and valleys is unique. In [8], a linear algorithm (Algorithm MHS) was proposed for determining a perfect path system for a hexagonal system, which means that we can determine the induced matching between peaks and valleys in a linear time. Let $\mu(H)$ be this induced matching, *i.e.*, $(p, v) \in \mu(H)$ if and only if p and v are the ends of a monotone path in some perfect path system. Below, we always assume that if $(p, v) \in \mu(H)$ then p is a peak and v is a valley. For a given $(p, v) \in \mu(H)$, let $R_{p,v}$ (resp. $L_{p,v}$) denote the rightmost (resp. leftmost) monotone path from p to v which is also contained in a perfect path system. All $R_{p,v}$'s (resp. $L_{p,v}$'s) together form a perfect path system of H [7] which is called the *right* (resp. *left*) *path system* (see Fig. 4), denoted by $\mathcal{R}$ (resp. $\mathcal{L}$). Linear algorithms (Routines RPS and LPS) based on Algorithms MHS were given in [7] to find $\mathcal{R}$ and $\mathcal{L}$. Let v be a vertex of H which is incident to three edges, say x, y, z. We have three ways to embed H in the plane such that x, y, z are vertical edges respectively (we do not distinguish between positions obtainable from each other by a rotation of 180^0). Different embeddings have different peaks and valleys. Thus the corresponding $\mu(H)$, $\mathcal{R}$, $\mathcal{L}$ are also different. Hence, in the following we use x, y, z to be subscripts to distinguish them.

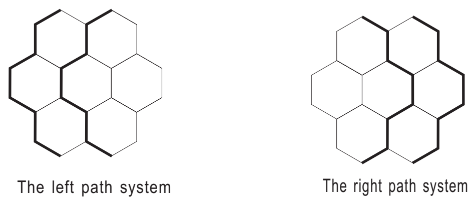


Fig. 4. Illustration for the left and right path systems.

Let P be a monotone path from a peak to a valley in H. Then the subgraph $H-V(P)$ may have several connected components. A *left* (*right*) *bank* of P consists of all the left (right) components of $H-V(P)$, the edges between P and these components, and P itself.

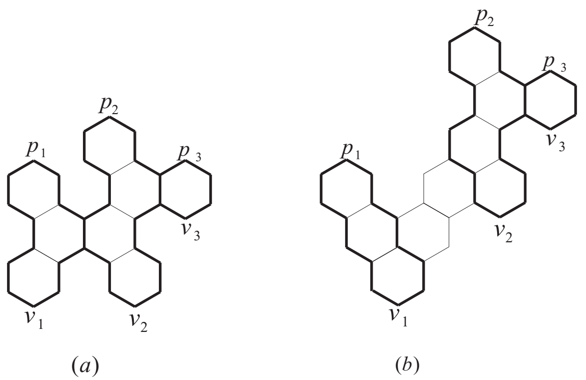


Fig. 5. (a) $G(H)$ with one maximal cycle; (b) $G(H)$ with two maximal cycles.

Let $R_{p,v} \oplus L_{p,v}$ be the set of edges which belong to $R_{p,v}$ or $L_{p,v}$ but not to both. Let $G(H)$ be the union of all $R_{p,v} \oplus L_{p,v}$ (see Fig. 5). A *maximal cycle* of $G(H)$ is a cycle which is not contained in the region bounded by another cycle of $G(H)$. Any two maximal cycles are disjoint. If C is a cycle of H, we denote the subgraph system of H with C as its boundary by $I[C]$.

The following lemma provides an efficient criterion to determine whether or not a given edge e of H is a fixed edge in terms of $G(H)$.

Lemma 3.1. *[7] An edge e of H is not a fixed edge if and only if there is some maximal cycle C of $G(H)$ such that $e \in E(I[C])$.*

As an immediate consequence of the above lemma, we have the following interesting property of normal hexagonal systems.

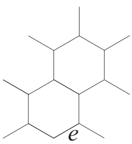
Corollary 3.2. *Let H be a normal hexagonal system. Then for any $(p, v) \in \mu(H)$, $E(R_{p,v} \cap L_{p,v}) = \emptyset$. Moreover, $G(H)$ has only one maximal cycle which is the boundary of the exterior face.*

Proof. Suppose, to the contrary, that there is an edge $e \in E(R_{p,v} \cap L_{p,v})$. Since for any monotone path P from p to v which is contained in some perfect path system, P is between $R_{p,v}$ and $L_{p,v}$, we have $e \in P$. If e is non-vertical, then e is in all perfect matchings of H, otherwise it is in none of perfect matchings of H. In either case, e is a fixed edge. This is a contradiction.

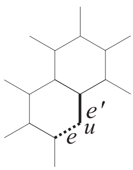
If $G(H)$ has at least two maximal cycles, since any two maximal cycles of $G(H)$ are disjoint, the edges connecting any two maximal cycles are not in any maximal cycle. By Lemma 3.1, such edges are fixed edges, which is a contradiction. Moreover, the only maximal cycle of $G(H)$ has to be the boundary of the exterior face, otherwise the edges which are not contained in the interior region of the maximal cycle are fixed edges, a contradiction. ■

Since $R_{p,v}$ and $L_{p,v}$ have the same end vertices, by Corollary 3.2, we can know that $R_{p,v} \oplus L_{p,v}$ is a cycle.

Let H be a normal hexagonal system without any (2, 3, 2) path. Then the anti-Kekulé number of H may be 2 or 3. In the following, we want to determine whether the anti-Kekulé number of H is 2 or not. Note that if $\{e, f\}$ is an anti-Kekulé set of H, then f is a fixed double edge of $H - e$. Hence we need a criterion to determine if an edge is a fixed edge of $H - e$.



(a)



(b)

Fig. 6. Edge e of a hexagonal system H

For $e \in E(H)$, embed H in the plane such that e is non-vertical. If both end vertices of e are of degree 3 or e has only one end vertex of degree 2 which is a peak or a valley of H (see Fig. 6(a)), then $H - e$ has the same peaks and valleys as H. If e has one end vertex u of degree 2 which is neither a peak nor a valley, then the other edge of H which is incident with u, say $e^{'}$, is a vertical edge (see Fig. 6(b)). Clearly, $e^{'}$ is a fixed double edge of $H - e$. Since H has no (2, 3 , 2) paths, deleting $e^{'}$ and its end vertices from $H - e$ does not generate new peaks and valleys. Thus the remaining subgraph has the same peaks and valleys as H. Consequently, although all neighbors of u are below or above it, we can overlook u and define the peaks and valleys of $H - e$ as those of H. In either case, there is a one-to-one correspondence between perfect matchings and perfect path systems of $H - e$. Moreover, the induced matching between the peaks and valleys of $H - e$ is unique. Define the left, the right path systems and $G(H - e)$ for $H - e$ in the same way as those of H. In the following, we always assume that $L^{'}_{p,v}$ (resp. $R^{'}_{p,v}$) is the new leftmost (resp. rightmost) monotone path from p to v which is contained in a perfect path system of $H - e$. In [9], it was pointed out that all the results of [7] can be extended from H to $H - e$. In particular, the following conclusion holds which will provide an efficient criterion to determine whether or not a given edge is a fixed edge in $H - e$.

Lemma 3.3. *[9] An edge of $H - e$ is not fixed if and only if there is a maximal cycle C of $G(H - e)$ such that the edge is contained in $I[C]$.*

For $e \in G(H)$, if $e \in L$ (resp. R) of $\mathcal{L}$ (resp. $\mathcal{R}$), then some leftmost (resp. rightmost) monotone paths of H in the right (resp. left) bank of L (resp. R) may need to shift right (resp. left) to be the new leftmost (resp. rightmost) monotone paths in $H - e$. This means that there may be some $(p, v) \in \mu(H - e)$, such that $E(L^{'}_{p,v} \cap R_{p,v}) \neq \emptyset$ or $E(L_{p,v} \cap R^{'}_{p,v}) \neq \emptyset$. For any edge of $E(L^{'}_{p,v} \cap R_{p,v})$ or $E(L_{p,v} \cap R^{'}_{p,v})$, it is not contained in the interior region of any maximal cycle of $G(H - e)$. Besides, if e has one end vertex u of degree 2 which is neither a peak nor a valley, let $e^{'}$ be the vertical edge incident with u. Then $e^{'}$ and all the edges adjacent to $e^{'}$ are also not contained in the interior region of any maximal cycle of $G(H - e)$. On the other hand, for any edge not as the edge of the two cases mentioned above, it must be contained in $E(L^{'}_{p,v} \cap R_{p,v})$ or $E(L_{p,v} \cap R^{'}_{p,v})$ for some $(p, v) \in \mu(H - e)$, which implies that it is contained in the interior region of some maximal cycle of $G(H - e)$. Hence an edge is not contained in the interior region of some maximal cycle of $G(H - e)$ if and only if it is $e^{'}$, one of the edges adjacent to $e^{'}$ or one of the edges in $E(L^{'}_{p,v} \cap R_{p,v})$ or $E(L_{p,v} \cap R^{'}_{p,v})$. By Lemma 3.3, we know that:

Remark 3.4. *An edge is a fixed double edge of* $H-e$ *if and only if it is either the vertical edge intersecting* e *at a vertex of degree 2 or one of the non-vertical edges in* $E(L'_{p,v}\cap R_{p,v})$ *or* $E(L_{p,v}\cap R'_{p,v})$ *for some* $(p,v)\in\mu(H-e)$.

Lemma 3.5. *Let* H *be a normal hexagonal system. If* e *and* f *are two non-vertical edges which form an anti-Kekulé set of* H*, then* $e\in G(H)$ *and* $f\in G(H)$.

Proof. Suppose, to the contrary, that $e\notin G(H)$. Then in $H-e$, the left and the right path systems do not change. Thus, $G(H-e)=G(H)$. Since H is normal, by Corollary 3.2, the maximal cycle of $G(H)$ is the boundary of the exterior face of H, so does the maximal cycle of $G(H-e)$. By Corollary 3.3, $H-e$ has no fixed edges. But f is a fixed double edge of $H-e$. This is a contradiction. Therefore $e\in G(H)$. The discussion for the situation of $f\in G(H)$ is similar. Thus the statement holds. ■

Let $P=\{p_1,p_2,\ldots,p_k\}$, $V=\{v_1,v_2,\ldots,v_k\}$ be the sets of peaks and valleys of H respectively, $(p_i,v_i)\in\mu(H)$ $(i=1,2,\ldots,k)$. In the following, we abbreviate R_{p_i,v_i} (resp. L_{p_i,v_i}, R'_{p_i,v_i}, L'_{p_i,v_i}) by R_i (resp. L_i, R'_i, L'_i) $(i=1,2,\ldots,k)$. Let P_1, P_2 be two monotone paths from p to v which are contained in some perfect path system. If $P_1\oplus P_2$ is a cycle and $I[P_1\oplus P_2]$ is a linear hexagonal chain, then we say that P_1 (P_2) can *shift* to P_2 (P_1) by *one unit*, denoted by $P_1\xrightarrow{1}P_2$ (see Fig. 7).

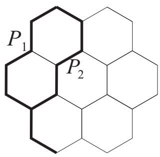


Fig. 7. $I[P_1\oplus P_2]$ is a hexagonal chain with 2 hexagons.

Lemma 3.6. *Let* H *be a normal hexagonal system,* e *a non-vertical edge of* R_i*. In* $H-e$*, if* $R'_j\neq R_j$*, then* $R_j\xrightarrow{1}R'_j$ *for* $j=1,2,\ldots,k$.

Proof. We distinguish two cases according to j=i or not.

Case 1. $j=i$.

If $e=wb\in R_i$ is as shown in Fig. 8(a), then let $e'=w'b'\in R_i$ be the first non-vertical edge which is above e and not parallel to e, P^R be the sub-path of R_i with b', w as its end vertices. If $e=wb\in R_i$ is as shown in Fig. 8(b), then let $e'=w'b'\in R_i$ be the first

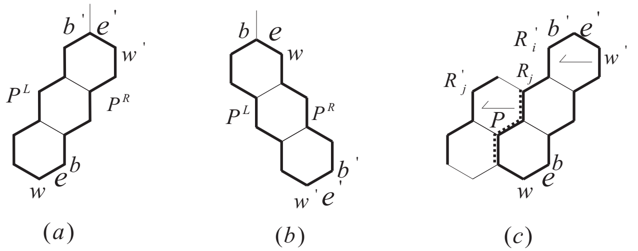


Fig. 8. Illustration for the proof of Lemma 3.6.

non-vertical edge which is below e and not parallel to e, P^R be the sub-path of R_i with b, w' as the end vertices. In either case, there is a linear hexagonal chain in $I[R_i \oplus L_i]$ along P^R. Denote the path on the left side of the chain by P^L. Let $P_i = R_i - P^R + P^L$. Then P_i is a monotone path from p_i to v_i. Let $\mathcal{A}$ be the subset of $\mathcal{L}$ which contains all the monotone paths in the left bank of L_i except L_i and $\mathcal{B}$ be the subset of $\mathcal{R}$ which contains all the monotone paths in the right bank of R_i except R_i. All the monotone paths in $\mathcal{A} \cup \{P_i\} \cup \mathcal{B}$ are disjoint and cover all peaks and valleys. Then $\mathcal{A} \cup \{P_i\} \cup \mathcal{B}$ is a perfect path system which contains P_i. Clearly P_i is the rightmost monotone path from p_i to v_i in $H - e$. Hence $R_i' = P_i$. Therefore $I[R_i \oplus R_i']$ is a linear chain. Thus $R_i \xrightarrow{1} R_i'$.

Case 2. $j \neq i$.

Note that for any $R_j \in \mathcal{B}$, R_j does not change in $H - e$, then $R_j = R_j'$. If all paths of $\mathcal{R} - \mathcal{B} - \{R_i\}$ do not intersect R_i', then they do not change in $H - e$. Hence the statement holds. If there is a path of $\mathcal{R} - \mathcal{B} - \{R_i\}$, say R_j, such that $E(R_i' \cap R_j) \neq \emptyset$. Note that $R_i' \cap R_j$ is a path, say P (see Fig. 8(c)). To avoid P, R_j needs to shift left. Since P consists of edges of at most two directions, there is a linear hexagonal chain along P and on the left side of P. Shift R_j to pass the left side of the chain we can get R_j'. Consequently, $R_j \xrightarrow{1} R_j'$. If R_j' intersects some rightmost paths of H in the left bank of R_j, then we can go on with the above procedure and eventually deduce the statement. ■

Remark 3.7. *If the shift $R_j \xrightarrow{1} R_j'$ is triggered by the shift $R_i \xrightarrow{1} R_i'$, then by the proof of Lemma 3.6, we can get more facts:*

(1)*$I[R_j \oplus R_j']$ is parallel to $I[R_i \oplus R_i']$ (we say two linear hexagonal chains are parallel if the two lines which join the centers of all hexagons of each chain are parallel),*

(2)*the range of $I[R_j \oplus R_j']$ is contained in the range of $I[R_i \oplus R_i']$,*

(3)*$|E(L_j \cap R_j')| \leq |E(L_i \cap R_i')|$.*

Remark 3.8. *For the non-vertical edge in some leftmost path, we can also have the similar results as Lemma 3.6 and Remark 3.7.*

4 Normal hexagonal systems H with $ak(H) = 2$

Let $d(u, v)$ be the distance between vertices u and v. The distance between two edges $e_i = u_iv_i$ and $e_j = u_jv_j$ of H, denoted by $d(e_i, e_j)$, is defined by $min\{d(u_i, u_j), d(u_i, v_j), d(v_i, u_j), d(v_i, v_j)\}$. In particular, we say e_i is at *distance one* from e_j if $d(e_i, e_j) = 1$. For any non-vertical edge e, there are at most 8 edges which are at distance one from it. Among these 8 edges, there is at most one non-vertical edge which is on the right side of e and connected to e by a non-vertical edge (see Fig. 9). If such an edge exists, then we denote it by f_e. Note that f_e is parallel to e.

Fig. 9. Illustration for e and f_e.

In the next theorem, we will characterize the normal hexagonal system whose anti-Kekulé number is two.

Theorem 4.1. *Let H be a normal hexagonal system. Then $ak(H) = 2$ if and only if H has a (2, 3, 2) path or an embedding satisfying the following two conditions:*
(a) There is a non-vertical edge e of $L_{p,v}$ for some $(p, v) \in \mu(H)$ such that $f_e \in R_{p,v}$,
(b) Let the opposite edges of e and f_e which are contained in $I[L_{p,v} \oplus R_{p,v}]$ be e^r and f_e^l respectively (see Fig. 9). Then $e^r \in R_{p,v}$, $f_e^l \in L_{p,v}$ or $e^r \in R_{p,v}$ and one of e, e^r is an inner edge or $f_e^l \in L_{p,v}$ and one of f_e, f_e^l is an inner edge.

Proof. Sufficiency. If H has a (2, 3, 2) path, then by Proposition 2.3, $ak(H) = 2$.

If H has an embedding satisfying conditions (a) and (b). Without loss of generality, let e, f_e be as shown in Fig. 9(a). Since $e \in L_{p,v}$ (resp. $f_e \in R_{p,v}$), we know that $L_{p,v}$ (resp. $R_{p,v}$) passes the two vertical edges adjacent to e (resp. f_e).

If $e^r \in R_{p,v}$, $f_e^l \in L_{p,v}$, then in $H-e^r$, $R_{p,v}$ needs to shift left to be $R_{p,v}^{'}$. By Lemma 3.6, $R_{p,v}^{'}$ will pass f_e^l and e. Thus $f_e^l \in E(L_{p,v} \cap R_{p,v}^{'})$. Since f_e^l is non-vertical, by Remark 3.4, f_e^l is a fixed double edge of $H-e^r$. By Lemma 2.2, $H-\{e^r, f_e^l\}$ is connected. Hence, $\{e^r, f_e^l\}$ is an anti-Kekulé set of H. Then $ak(H) \leq 2$. By Proposition 2.3, we have $ak(H)=2$.

If $e^r \in R_{p,v}$, then in $H-e^r$, $R_{p,v}$ needs to shift left to be $R_{p,v}^{'}$. Hence $R_{p,v}^{'}$ will pass e. Then e is a fixed double edge of $H-e^r$. If one of e and e^r is an inner edge, by Lemma 2.2, $H-\{e, e^r\}$ is connected. Hence $ak(H)=2$.

If $f_e^l \in L_{p,v}$ and one of f_e, f_e^l is an inner edge, then by a similar argument, we can also know that f_e^l is a fixed double edge of $H-f_e$ and $H-\{f_e, f_e^l\}$ is connected. Consequently, $\{f_e, f_e^l\}$ is an anti-Kekulé set of H. Hence $ak(H)=2$.

Necessity. Suppose $\{e_1, e_2\}$ is an anti-Kekulé set of H. Embed H in the plane with e_1, e_2 non-vertical. By Lemma 3.5, we know that $e_1 \in G(H)$, $e_2 \in G(H)$. Without loss of generality, let $e_1 \in R_i$. Then by Lemma 3.6, $R_i \xrightarrow{1} R_i^{'}$. Since e_2 is a non-vertical fixed double edge of $H-e_1$, there is a $(p,v) \in \mu(H)$ such that $e_2 \in E(L_{p,v}^{'} \cap R_{p,v}^{'})$. If e_1 is not in any leftmost monotone path in the right bank of R_i, then all the leftmost and the rightmost monotone paths in the right bank of R_i (except R_i) do not change. This implies that e_2 can only be in the left bank of R_i. If e_1 is in some leftmost monotone path in the right bank of R_i, then e_2 may be in the left bank or the right bank of R_i. By Remark 3.8, we can only discuss the former situation here. The discussion for the latter situation is similar. Hence in the following, we assume that e_2 is in the left bank of R_i. Since all the leftmost monotone paths in the left bank of R_i do not change, $e_2 \in E(R_{p,v}^{'} \cap L_{p,v})$ for some $(p,v) \in \mu(H)$. Since e_2 is non-vertical, it follows that $t=|E(R_{p,v}^{'} \cap L_{p,v})| \geq 2$.

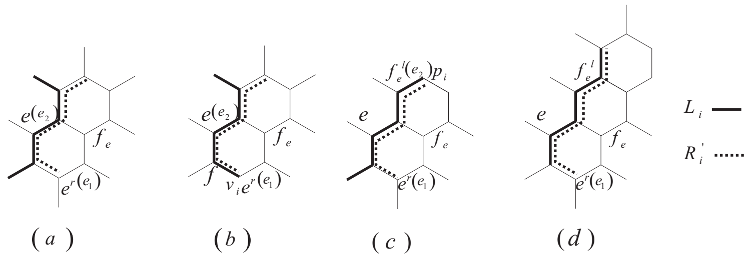


Fig. 10. Illustration for Case 1 in the proof of Theorem 4.1.

Case 1. $(p,v)=(p_i,v_i)$. Without loss of generality, let e_1 be as shown in Fig. 10(a).

Subcase 1.1. $t = 2$. Then e_2 is adjacent to e_1. Since $e_2 \in L_i$, $e_1 \in R_i$, both e_1 and e_2 are incident with v_i. Thus $H - \{e_1, e_2\}$ is disconnected, a contradiction.

Subcase 1.2. $t = 3$. Then e_2 is the only one non-vertical edge which is the opposite edge of e_1 in a hexagon of $I[R_i \oplus L_i]$ (see Fig. 10(a)). Since $H - \{e_1, e_2\}$ is still connected, by Lemma 2.2, it follows that one of e_1 and e_2 is an inner edge. Let $e = e_2$, $e^r = e_1$ and f_e be the first non-vertical edge of R_i above e_1 (see Fig. 10(a)). Then $d(e, f_e) = 1$, $f_e \in R_i$ and one of e and e^r is an inner edge. Hence conditions (a) and (b) hold.

Subcase 1.3. $t = 4$. Then $E(R_i^{'} \cap L_i)$ has two non-vertical edges, one is the opposite edge of e_1 in a hexagon of $I[R_i \oplus L_i]$, the other one, say f, is incident with p_i or v_i. If f is incident with v_i (see Fig. 10(b)), then e_2 cannot be f, otherwise $H - \{e_1, e_2\}$ is disconnected. Hence e_2 is the opposite edge of e_1 in a hexagon of $I[R_i \oplus L_i]$. Then by a similar argument as the proof of Subcase 1.2, we know that conditions (a) and (b) hold. If f is incident with p_i (see Fig. 10(c)), then let $e^r = e_1$, $f_e^l = f$ and e be the opposite edge of e_1 in a hexagon of $I[R_i \oplus L_i]$ (see Fig 10(c)). Hence conditions (a) and (b) hold.

Subcase 1.4. $t \geq 5$. Then there are at least two non-vertical edges in $R_i^{'} \cap L_i$. Let $e^r = e_1$, f_e be the first non-vertical edge of R_i above e_1, e be the opposite edge of e_1 in $I[R_i \oplus L_i]$. Then $d(e, f_e) = 1$, $f_e^l \in L_i$ and $e^r \in R_i$. Hence conditions (a) and (b) hold.

Case 2. $(p, v) = (p_j, v_j)$ $(j \neq i)$.

Subcase 2.1. $t = 2$. Then $R_j^{'} \cap L_j$ contains only one fixed double edge which is incident with p_j or v_j. Hence e_2 is incident with p_j or v_j. Without loss of generality, suppose that e_2 is incident with v_j. Note that the shift $R_j \xrightarrow{1} R_j^{'}$ is triggered by some shift, say $R_{j+1} \xrightarrow{1} R_{j+1}^{'}$. Then by Remark 3.7, the range of $I[R_j \oplus R_j^{'}]$ is contained in the range of $I[R_{j+1} \oplus R_{j+1}^{'}]$ and the two hexagonal chains are parallel. Since $d(v_j) = 2$, the lowest hexagons of $I[R_j \oplus R_j^{'}]$ and $I[R_{j+1} \oplus R_{j+1}^{'}]$ are adjacent and intersect at a vertical edge (see Fig. 11(a)). Let the lowest vertex of $I[R_{j+1} \oplus R_{j+1}^{'}]$ be v. Since $v_j \in L_j$, it follows that $v \in L_{j+1}$. Consequently, $v \in L_{j+1} \cap R_{j+1}$, which implies that v is a valley. Then we can obtain a (2, 3, 2) path.

Subcase 2.2. $t \geq 3$. Since $R_i \xrightarrow{1} R_i^{'}$ is the first shift, we have that $|E(L_i \cap R_i^{'})| \geq |E(L_j \cap R_j^{'})| \geq 3$. Without loss of generality, let e_1 be as shown in Fig. 11(b). Let $e^r = e_1$, f_e be the first non-vertical edge of R_i above e^r, and e be the opposite edge of e^r in $I[L_i \oplus R_i]$. Then $d(e, f_e) = 1$ and $e \in E(L_i \cap R_i^{'})$. Since $I[R_j \oplus R_j^{'}]$ is parallel to $I[R_i \oplus R_i^{'}]$ and the range of former is contained in the range of the latter, it follows that e is an inner edge (see Fig. 11(b)). Hence, conditions (a) and (b) hold. ∎

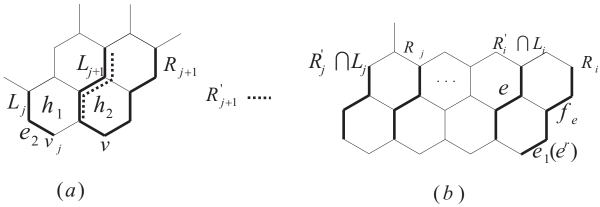


Fig. 11. Illustration for Case 2 in the proof of Theorem 4.1.

Benzenoid parallelogram $B_{p,q}$ is a hexagonal system which consists of $p \times q$ hexagons, arranged in q rows, each row consisting of p hexagons. Note that if $B_{p,q}$ has at least two hexagons, then $B_{p,q}$ has a (2, 3, 2) path. By Theorem 4.1, we can obtain the following result.

Corollary 4.2. *[17]* $ak(B_{p,q}) = 2$, *where* $pq \neq 1$.

A hexagon of a cata-condensed hexagonal system is said to be a *branched hexagon* if there are three hexagons adjacent to it. A cata-condensed hexagonal system is a *less-branched hexagonal system* if it has two adjacent non-branched hexagons. Otherwise, it is a *more-branched hexagonal system.* For instance, the graph G_2 shown in Fig. 2 is a more-branched hexagonal system.

Corollary 4.3. *If* H *has no (2, 3, 2) paths and* $ak(H) = 2$. *Then* H *is not a more-branched hexagonal system.*

Proof. By Theorem 4.1, H has an embedding satisfying conditions (a) and (b). Let e, f_e, e^r and f_e^l be as Theorem 4.1 defined and as shown in Fig. 12(a). Let h_1, h_2 be the two hexagons of H containing these four edges (see Fig. 12(a)).

Claim 1. If $f_e^l \in L_i$ and there is a hexagon h_3 such that $h_3 \cap h_1 = f_e^l$, then H is a pericondensed hexagonal system.

Since $e \in L_i$, $f_e^l \in L_i$, there is $(p_j, v_j) \in \mu(H)$ such that $j \neq i$ and $h_3 \subset I[L_j \oplus R_j]$. Then e is contained in another hexagon different from h_2, otherwise $L_j \cap L_i \neq \emptyset$. Hence H is pericondensed.

Claim 2. If $e^r \in R_i$ and there is a hexagon h_4 such that $h_4 \cap h_2 = e^r$, then H is a pericondensed hexagonal system.

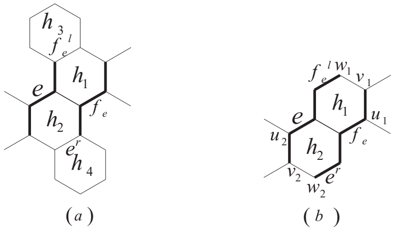


Fig. 12. Illustration for the proof of Corollary 4.3.

By a similar argument as Claim 1, we can deduce that f_e is contained in another hexagon different from h_1. Hence H is pericondensed.

There are three cases in condition (b) of Theorem 4.1.

Case 1. $f_e^l \in L_i$ and $e^r \in R_i$.

If H is pericondensed, then H cannot be a more-branched hexagonal system. If H is cata-condensed, then both of e and f_e are peripheral. By Claims 1 and 2, both of e^r and f_e^l are peripheral. Label some vertices of h_1 and h_2 as shown in Fig. 12(b). Since H has no (2, 3, 2) paths, u_1v_1 (u_2v_2) is not peripheral and thus contained in another hexagon different from h_1 (h_2). Since H is cata-condensed, both of w_1v_1 and w_2v_2 are peripheral. Then h_1 and h_2 are two adjacent non-branched hexagons of H, which implies that H cannot be a more-branched hexagon system.

Case 2. $e^r \in R_i$ and one of e, e^r is an inner edge.

If e^r is inner, by Claim 2, H is pericondensed. If e is inner, then H is also pericondensed.

Case 3. $f_e^l \in L_i$ and one of f_e, f_e^l is an inner edge.

If f_e^l is inner, by Claim 1, H is pericondensed. If f_e is inner, then H is also pericondensed. ■

Corollary 4.4. *[18] Let H be a cata-condensed hexagonal system. If H is a more-branched hexagonal system, then $ak(H) = 3$. Otherwise $ak(H) = 2$.*

Proof. If H is a more-branched hexagonal system, then H has no (2, 3, 2) paths, otherwise H has two adjacent non-branched hexagons. Hence, by Corollary 4.3, $ak(H) = 3$. If H is a less-branched hexagonal system, then H has two adjacent non-branched hexagons, say h_1 and h_2. Without loss of generality, suppose that h_1 intersects h_2 at a vertical edge. If H has a (2, 3, 2) path in $h_1 \cup h_2$, then $ak(H) = 2$. If $h_1 \cup h_2$ has no (2, 3, 2) paths, then h_1, h_2 can only be as shown in Fig. 13(a) or (b). Without loss of generality, let they be as shown in Fig. 13(b). Let u_1v_1 (resp. u_2v_2) be the edge of h_1 (resp. h_2) whose two end vertices are of degree two. Rotate H 120^0 in a clockwise direction such that H is as shown in Fig. 13(c). Then u_1 is a peak and v_2 is a valley. Let $(u_1, v) \in \mu(H)$. Since $h_1 \subset I[L_{u_1,v} \oplus R_{u_1,v}]$, h_2 belongs to $I[L_{u_1,v} \oplus R_{u_1,v}]$. Then $v = v_2$. Hence $u_1v_1 \in L_{u_1,v}$ and $u_2v_2 \in R_{u_1,v}$. By Theorem 4.1, $ak(H) = 2$. ■

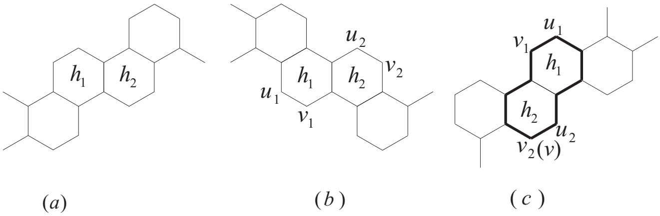


Fig. 13. Illustration for the proof of Corollary 4.4.

5 An algorithm

Based on Theorem 4.1, we can now give an algorithm for finding a smallest anti-Kekulé set in a normal hexagonal system.

Algorithm AKS.

Input: A normal hexagonal system H.

Output: A smallest anti-Kekulé set K of H.

Step 1: Mark all the edges in $\partial(H)$ which is the boundary of H. If $\partial(H)$ has a path uvw such that $d(u) = d(w) = 2$ and $d(v) = 3$ in H respectively, then return that $K = \nabla(\{u, w\}) - \{uv, vw\}$. Otherwise, choose a path uvw such that $d(u) = 2$ and $d(v) = d(w) = 3$ in H respectively. Let $K = \nabla(\{u, w\}) - \{uv, vw\}$, go to Step 2.

Step 2: Determine $\mu_x(H)$, $\mu_y(H)$, $\mu_z(H)$ by Algorithm MHS. Let $\mathcal{S}$=$\{\mu_x(H), \mu_y(H), \mu_z(H)\}$.

Step 3: **while** $\mathcal{S} \neq \emptyset$, **do**

choose $\mu(H) \in \mathcal{S}$. Determine $\mathcal{L}$, $\mathcal{R}$ by Routines LPS and RPS.

for $(p, v) \in \mu(H)$, **do**

mark the edges which belong to $L_{p,v} \oplus R_{p,v}$. Let E be the set of non-vertical edges in $L_{p,v}$.

for $e \in E$, **do**

if $f_e \notin R_{p,v}$, **then** delete e from E.

else mark f_e.

(a) **if** $e^r \in R_{p,v}$, $f_e^l \in L_{p,v}$, **then** return that $K = \{e^r, f_e^l\}$.

(b) **if** $e^r \in R_{p,v}$ and one of e and e^r does not belong to $\partial(H)$,

then return that $K = \{e, e^r\}$.

(c) **if** $f_e^l \in L_{p,v}$ and one of f_e and f_e^l does not belong to $\partial(H)$,

then return that $K = \{f_e, f_e^l\}$.

end for

end for

end while

Return K.

Finding the anti-Kekulé sets of the two graphs G_1 (see Fig. 2) and G_3 (see Fig. 14) are two applications of this algorithm. It can be seen that both of the two graphs have no (2, 3, 2) paths. For the embedding of G_1 shown in Fig. 2, mark its peaks and valleys as p_i and v_i $(i = 1, 2, \ldots, 8)$. We can determine $L_i \oplus R_i$ and find that the non-vertical edges of L_1 and L_2 do not satisfy cases (*a-c*) in Algorithm AKS. For (p_3, v_3), we can verify that e, $f_e^l \in L_3$, f_e, $e^r \in R_3$, and $d(e, f_e) = 1$. Hence all of $\{e^r, f_e^l\}$, $\{e, e^r\}$, $\{f_e, f_e^l\}$ are anti-Kekulé sets of G_1. For the three embeddings of the graph G_3 shown in Fig. 14, mark their peaks and valleys, determine their left and right path systems. We can find that for any non-vertical edge e of any leftmost monotone path, its corresponding edges e^r, f_e and f_e^l do not satisfy cases (*a-c*) in Algorithm AKS. Hence $ak(G_3) = 3$ and $\nabla(\{u, w\}) - \{uv, vw\}$ is an anti-Kekulé set of size three in G_3.

Theorem 5.1. *Algorithm AKS finds a smallest anti-Kekulé set in a normal hexagonal system H correctly in an $O(n^2)$ time, where n is the number of verices of H.*

Proof. The correctness of the Algorithm AKS is guaranteed by Theorem 4.1. Hence we just need to do the complexity analysis. Since $\partial(H)$ contains at most $2n$ edges, and since Algorithm MHS can be done in O(n) time, Steps 1 and 2 take O(n) time. In Step 3, since Routines LPS, RPS can be done in O(n) time, we can determine $\mathcal{L}$, $\mathcal{R}$ in O(n) time. For $(p, v) \in \mu(H)$, we search along $L_{p,v}$ and $R_{p,v}$ once and mark all the edges in $L_{p,v} \oplus R_{p,v}$.

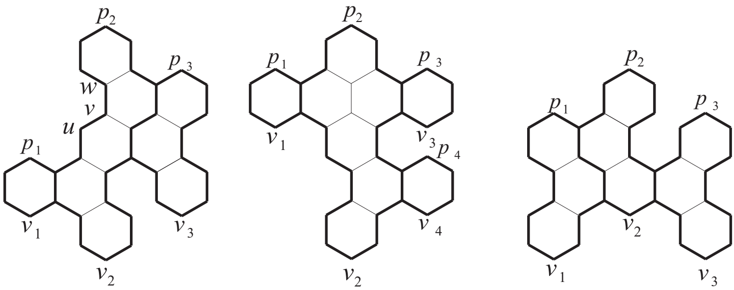


Fig. 14. Three embeddings of G_3 in the plane.

Since $\mathcal{L}$ and $\mathcal{R}$ are perfect path systems of H, they contain at most $2n$ edges. Thus this task will take O(n) time. Since H is normal, by Corollary 3.2, $L_{p,v} \oplus R_{p,v} = L_{p,v} \cup R_{p,v}$. Hence the edges of $R_{p,v} \cup L_{p,v}$ had been marked. Note that the edges of $\partial(H)$ had also been marked. Then for each non-vertical edge of $L_{p,v}$, it takes constant time to test whether or not e, e^r, f_e and f_e^l satisfy cases(*a*-*c*) in Algorithm AKS. Since $\mathcal{L}$ contains at most $\frac{n}{2}$ non-vertical edges, we do the testing work at most $\frac{n}{2}$ times. Hence for each $(p, v) \in \mu(H)$, the algorithm takes us O(n) time. For each $\mu(H) \in \mathcal{S}$, $\mu(H)$ contains at most $\frac{n}{2}$ pairs of (p, v), which means that we do the task of marking and testing edges at most $\frac{n}{2}$ times. Hence for each $\mu(H) \in \mathcal{S}$, the algorithm takes us at most O(n^2) time. Since $|\mathcal{S}| = 3$, the overall time complexity of Step 3 is O($3n^2$)=O(n^2). By the above results, the complexity of Algorithm AKS is O(n^2). ■

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