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Algebraic Kekulé Structures of Constructable Hexagonal Systems*

Xin He, Heping Zhang†

School of Mathematics and Statistics, Lanzhou University, Lanzhou, Gansu 730000, P. R. China

hex2015@lzu.edu.cn, zhanghp@lzu.edu.cn

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Abstract

An algebraic Kekulé structure (AKS) of a hexagonal system H corresponding to a geometric Kekulé structure (GKS) is a function from the hexagons to integers which describe the π-electrons distribution within rings of benzenoid hydrocarbons. Gutman et al. (2004) showed that all catacondensed hexagonal systems with at least 2 hexagons have a one-to-one correspondence between GKS and AKS. It is natural to consider which pericondensed hexagonal systems have such one-to-one correspondence. In this paper, we characterize the constructable hexagonal system (CHS) with a one-to-one correspondence between GKS and AKS. As applications to parallelograms, truncated parallelograms and chevrons, and multiple chains, among them we determine all several graphs without the above one-to-one correspondence.

1 Introduction

A hexagonal system (HS, or benzenoid) is a 2-connected finite plane graph such that every interior face is a regular hexagon. A matching of a graph G is a set of pairwise disjoint edges. A matching is called a perfect matching if it covers all the vertices of G. We are interested in the hexagonal systems with a perfect matching, which can be regarded as the carbon skeleton of benzenoid hydrocarbon molecules. A perfect matching

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†Corresponding author.

of an HS is also called geometric Kekulé structure (GKS). About 15 years ago, Randić [13, 14] introduced algebraic Kekulé structure (AKS) of an HS from a GKS K, which is a function from hexagons to integers according to the following rule: every edge in K which belongs to only one hexagon contributes 2 to the function value of this hexagon and every edge in K shared by two hexagons contributes 1 to each one of these two hexagons. The function values on hexagons are called the Randić numbers, which are ranging from 0 to 6. The AKS was originally used for the coding and ordering of GKS of some benzenoid hydrocarbons [12–14, 18] and further employed to assess the π-electron contents of rings in them in chemistry [1–5, 8, 9, 15].

With regards to coding and computer-aided processing, AKS has an obvious advantage over the GKS [12, 18]. In view of this, it is of primary interest to establish a one-to-one correspondence between them. Obviously, every GKS uniquely determines an AKS, but the opposite is not true [4, 10, 17].

An HS is said to be *catacondensed* if no three of its hexagons have a vertex in common, and *pericondensed* otherwise. It was shown by Gutman et al. [10] that there exists a one-to-one correspondence between GKSs and AKSs of each catacondensed HS with at least 2 hexagons. However, the correspondence between GKS and AKS of a pericondensed HS is more complicated. As we know, Vukičević et al. [17] gave a characterization for an HS to have more GKSs than AKSs (see the next section). Using this result, Y. Zhang and H. Zhang [21] obtained the following two types of HSs with at least two hexagons that have a one-to-one correspondence between GKS and AKS: benzenoid parallelogram $P(p, q)$ except $P(2, 2)$, consisting of $p \times q$ hexagons arranged in p rows and q columns, and any HSs with no $P(2, 2)$ as its subgraph.

In this paper, we characterize the constructable HSs that have a one-to-one correspondence between GKS and AKS. For simplicity, we call an HS H *singular* if H does not have a one-to-one correspondence between GKS and AKS, and *nonsingular* otherwise. In Section 2, we give some further properties of singular general CHSs. Based on these properties, in Sections 3 and 4 we obtain our main results that are sufficient and necessary conditions for monotonic CHSs and general CHSs to be singular, respectively. In Section 5, applying our results to special types of CHSs, such as parallelograms, truncated parallelograms and chevrons, and multiple chains, among them we determine all five singular graphs (single hexagon and $P(2, 2)$ for (truncated) parallelograms, two for truncated chevrons and one for multiple chains). Finally, we propose some problems on further researches in Section 6.

2 Preliminaries

For a graph G, the set of vertices of G is denoted by $V(G)$ and the set of edges by $E(G)$. For a subgraph G' of G, the graph induced by the set of vertices $V(G) \setminus V(G')$ will be denoted by $G - V(G')$. For matchings M_1 and M_2 of G, a cycle C of G is called (M_1, M_2)-alternating cycle if the edges of C appear between M_1 and M_2 alternatively. The symmetric difference of two sets S_1 and S_2 is denoted by $S_1 \oplus S_2 = (S_1 \cup S_2) \setminus (S_1 \cap S_2)$. For an HS H, an edge of H is called an *peripheral edge* if it belongs to the exterior face of H, and an *inner edge* otherwise. We denote the sets of inner edges and peripheral edges of H by $E_i(H)$ and $E_p(H)$ respectively. For a hexagon h of H and a matching M of H, let $AKS_h(M) = |E_i(h) \cap M| + 2|E_p(h) \cap M|$.

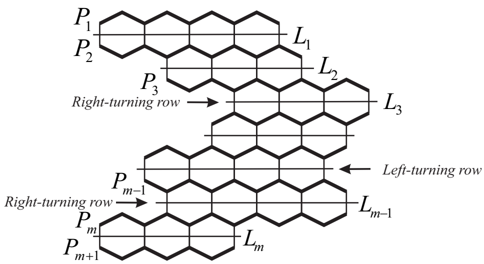


Figure 1. A constructable HS.

An HS is said to be a constructable HS (CHS) [6, 7, 19], if it can be drawn in the plane such that some edges are vertical and dissected by a series of parallel horizontal lines L_i $(i = 1, 2, \dots, m)$ into $m + 1$ *horizontal zigzag paths* $P_1, P_2, \dots, P_{m+1}$ so that the top P_1 and the bottom P_{m+1} must be of even length, and all other paths are of odd length (see Fig. 1). The CHS includes some special classes of HSs, such as parallelogram, truncated parallelogram and chevron, and multiple chain [6].

The following useful terms and notions about CHSs were introduced in [7]. We call the linear hexagonal chain which consists of all the hexagons intersecting L_i $(i = 1, 2, \dots, m)$ the i-th *row* R_i of H. If the up end-vertex of the most-left (resp. most-right) vertical edge of R_i $(i \geq 2)$ has degree 3, then we say that R_i turns to the right (resp. left). If the end vertices of the most-left (resp. most-right) vertical edge of R_i both have degree 3, then R_i is called a *right turning* (resp. *left turning*) row. Both right turning row and left turning row are called *turning rows*. If a CHS has no turning row, then it is called a *monotonic* CHS. More specifically, besides the top row, if each row of a CHS turns to the right (resp. left), then this CHS is called *right monotonic* (resp. *left monotonic*). By symmetry, left monotonic and right monotonic are equivalent. For more terms and notions we follow [6].

For convenience, we denote by $h_{1,1}$ the most-left hexagon on the top row of H and then define all other hexagons of H inductively. If $h_{i,j}$ is a hexagon of H, we denote by $h_{i,j+1}$, $h_{i+1,j}$, $h_{i+1,j-1}$ and $h_{i,j-1}$ the hexagons (if they exist) neighboring $h_{i,j}$ on the right, the bottom right, the bottom left and the left side respectively. Moreover, for a hexagon h of H we denote by $e_l(h)$, $e_{tl}(h)$, $e_{tr}(h)$, $e_r(h)$, $e_{br}(h)$ and $e_{bl}(h)$ the left vertical edge, the top left edge, the top right edge, the right vertical edge, the bottom right edge and the bottom left edge of h respectively.

We know that a CHS has at least one perfect matching with the following properties.

Lemma 2.1 ([19]). *Every perfect matching of a CHS H contains exactly one vertical edge of each row of H.*

Lemma 2.2 ([19]). *Let M be a perfect matching of a CHS H with m rows and e_i ($i = 1, 2, \ldots, m$) be the vertical edge of M in R_i of H. If R_i ($2 \leq i \leq m$) of H turns to the right (resp. left), then e_i is on the right (resp. left) of e_{i-1}.*

The following key theorem was obtained by Vukičević et al.

Theorem 2.3 ([17]). *An HS H is singular if and only if H contains a subgraph $\mathcal{C}$ that consists of at least one disjoint cycles and the edges of $\mathcal{C}$ can be divided into two matchings M_1 and M_2 such that the following three conditions are satisfied:*

(1) $M_1 \oplus M_2 = E(\mathcal{C})$,

(2) $H - V(\mathcal{C})$ has a perfect matching, and

(3) for each hexagon h of H, $AKS_h(M_1) = AKS_h(M_2)$.

It is obvious that the disjoint perfect matchings M_1 and M_2 of $\mathcal{C}$ in Theorem 2.3 can be extended to two perfect matchings M_1' and M_2' of H where $M_1' = M_1 \cup M_0$ and $M_2' = M_2 \cup M_0$ for a perfect matching M_0 of $H - V(\mathcal{C})$. We say an edge of M_0 is a *fixed matching edge relative to* $\mathcal{C}$. In the figure, we often use thick edges to denote the edges of $\mathcal{C}$, and double edges the fixed matching edges relative to $\mathcal{C}$.

To get our main results we now discuss some properties of $\mathcal{C}$ in Theorem 2.3. From now on we suppose that H is a singular hexagonal system, and that $\mathcal{C}$, M_1 and M_2 are the same as in Theorem 2.3 with the conditions (1), (2) and (3). A HS H is called *convex* if it does not have a peripheral edge with two end vertices of degree 3, and *concave* otherwise. The following two lemmas have already been obtained.

Lemma 2.4 ([21])**.** *For any hexagon h of H, $|E_i(h) \cap E(\mathcal{C})|$ is an even number.*

Lemma 2.5 ([21])**.** *If a cycle C of $\mathcal{C}$ does not contain another cycle of $\mathcal{C}$ in its interior, then C must bound a convex HS.*

Further, in the remaining part of this section we suppose that H is a CHS. In this situation we can see that the condition of Lemma 2.5 always holds. If a cycle C of $\mathcal{C}$ contains another cycle C^* in the interior of C, then there is some row intersecting both C and C^* at vertical edges. So M_1 and M_2 each contains at least two vertical edges of this row, because each of such two cycles has one vertical edge of M_i $(i = 1, 2)$ in this row. Since each of M_1 and M_2 can be extended to a perfect matching of H, it contradicts lemma 2.1. So from lemma 2.5 we have the following result.

Lemma 2.6. *The interiors of any two cycles of $\mathcal{C}$ are disjoint, and each row of H intersects at most one cycle of $\mathcal{C}$ in vertical edges. So each cycle of $\mathcal{C}$ bounds a convex HS.*

Lemma 2.7. *Any cycle C of $\mathcal{C}$ bounds a parallelogram $P(p, q)$ with $p, q \geq 1$.*

Proof. From lemma 2.6 a cycle C of $\mathcal{C}$ bounds a convex HS H' with a perfect matching M such that C is M-alternating. Then either H' is a linear chain or the second row of H' (if exists) turns to the right or the left. Otherwise, the second row of H' exists and has zero or two vertical edges in M (this can be easily obtained from Lemma 1 of [20] or the white-black coloring method of [16]). Since C is an M-alternating cycle, this row has at least one vertical edge in M. On the other hand, since a perfect matching of H' can be extended to a perfect matching of H, this row contains at most one vertical edge in M by lemma 2.1. Both imply that this row contains exactly one vertical edge in M, which is a contradiction. Continuing this way we can show that H' is also a CHS. Further, that H' is convex implies that H' a parallelogram $P(p, q)$ with $p, q \geq 1$. ■

From lemma 2.7 a cycle of $\mathcal{C}$ bounds a parallelogram or its degenerated cases: a single hexagon and a linear hexagonal chain. For convenience, for a cycle C in $\mathcal{C}$ the subgraph of H that consists of all hexagons of H in the interior of C and the hexagons of H that have an edge of C is called the *local structure* of C.

Lemma 2.8. *If a cycle C of $\mathcal{C}$ is a single hexagon h, then there are 6 possible local structures of C as shown in Fig. 2.*

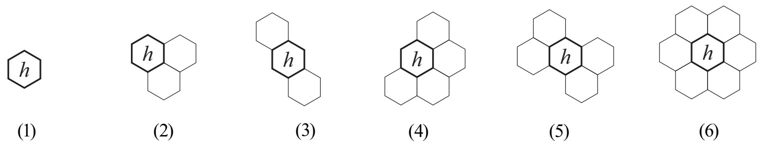


Figure 2. The local structures of a single hexagon h.

Proof. If a cycle C of $\mathcal{C}$ is a single hexagon h, then we know that $|E_i(h) \cap E(\mathcal{C})|$ is even by lemma 2.4. When $|E_i(h) \cap E(\mathcal{C})| = 0$, the only local structure of C is Fig. 2(1). When $|E_i(h) \cap E(\mathcal{C})| = 2$, Condition (3) of Theorem 2.3 shows that there are two local structures of h as shown in Fig. 2(2) and (3). Similarly, when $|E_i(h) \cap E(\mathcal{C})| = 4$, there are two local structures of C which are Fig. 2(4) and (5). For $|E_i(h) \cap E(\mathcal{C})| = 6$, the local structure of h can only be Fig. 2(6). ■

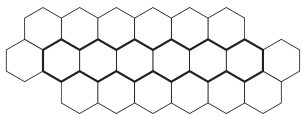


Figure 3. The local structure of C bounding a linear hexagonal chain.

Lemma 2.9. *If one cycle C of $\mathcal{C}$ bounds a linear hexagonal chain at least two hexagons, then there is only one local structure of C up to isomorphism in which C has exactly two peripheral edges as shown in Fig. 3.*

Proof. Let a cycle C of $\mathcal{C}$ be the boundary of a linear hexagonal chain of length at least two. Then all possible local structures of C have already been given in Claim 4.3 of Ref. [21]; see Fig. 4, where just one of hexagon i' and i'' ($1 \leq i \leq n-1$) in the first graph belongs to H.

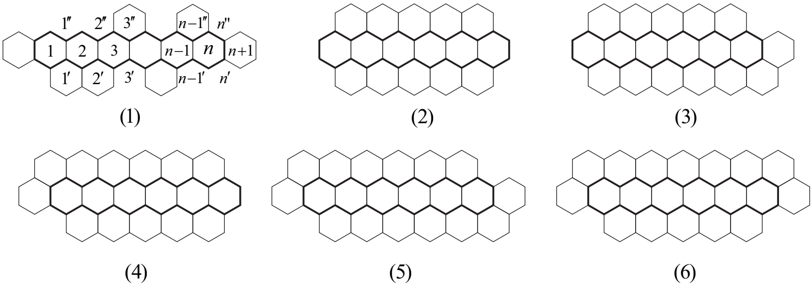


Figure 4. The possible local structures of C bounding a linear hexagonal chain.

It is sufficient to show that all possible local structures except (5) cannot be a subgraph of H. We only consider (3) (the others are similar). Since an HS has three different directions, the CHS H has three possible drawings in the plane such that each row is horizontal. So the local structure of C has also three corresponding drawings as Fig. 5 up to mirror reflections. For (a), the path P is of even length, which contradicts the definition

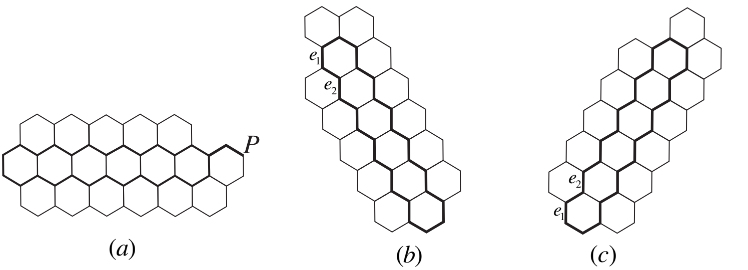


Figure 5. Three drawings for the local structure (3) of C.

of CHS. For (b), the vertical edges e_1 and e_2 belong to the same perfect matching of H, and the row including e_2 turns to left, but e_2 is on the right side of e_1, which contradicts lemma 2.2. For (c), the vertical edges e_1 and e_2 belongs to the same perfect matching of H, and the row including e_1 turns to the right, but e_1 is on the left side of e_2, a contradiction again. Hence the local structure (3) cannot be a subgraph of H. ■

Lemma 2.10. *If a cycle C of $\mathcal{C}$ bounds a parallelogram $P(p,q)$ with $p,q \geq 2$, then there is only one local structure of C up to isomorphism in which C has exactly two peripheral edges as shown in Fig. 6.*

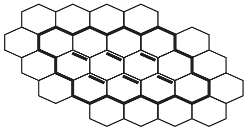


Figure 6. The local structure of C bounding a parallelogram.

Proof. Suppose that a cycle C of $\mathcal{C}$ is the boundary of a parallelogram $H' = P(p,q)$ with $p, q \geq 2$ (see Fig. 7). We can see that $H' - V(C)$ has only one perfect matching and there is no cycle of $\mathcal{C}$ inside C. All hexagons of H' and possible neighboring hexagons are labelled as Fig. 7. Applying lemma 2.4 and theorem 2.3 (3) to $h_{p,1}$, we find that $h_{p+1,0}$

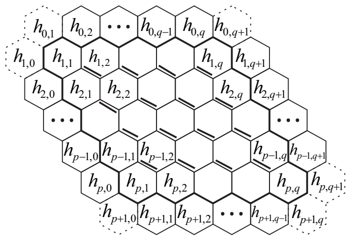


Figure 7. Illustration for the proof of lemma 2.10.

is not a hexagon of H and both $h_{p+1,1}$ and $h_{p,0}$ are hexagons of H. Applying lemma 2.4 to $h_{p,2}, h_{p,3}, \ldots, h_{p,q-1}$ successively, and to $h_{p-1,1}, h_{p-2,1}, \ldots, h_{2,1}$ successively, we find that $h_{p+1,2}, h_{p+1,3}, \ldots, h_{p+1,q-1}$ and $h_{p-1,0}, h_{p-2,0}, \ldots, h_{2,0}$ are hexagons of H. Similarly, we can show that $h_{1,q+1}, h_{2,q+1}, \ldots, h_{p-1,q+1}$ and $h_{0,q}, h_{0,q-1}, \ldots, h_{0,2}$ are hexagons of H, and $h_{0,q+1}$ is not a hexagon of H. Furthermore, applying lemma 2.4 to $h_{1,1}$ and $h_{p,q}$, we find that

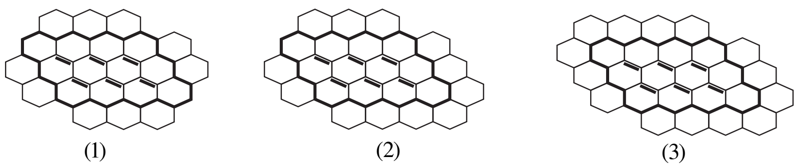


Figure 8. The possible local structures of C bounding a parallelogram.

both $h_{1,0}$ and $h_{0,1}$ are hexagons of H or not simultaneously, and both $h_{p,q+1}$ and $h_{p+1,q}$ are hexagons of H or not simultaneously. Therefore, there are total three possible local structures of C as shown in Fig. 8.

We can show that none of the first two is a subgraph of H by the same method as in the proof of lemma 2.9. ■

3 Monotonic constructable hexagonal system

Let H be a right monotonic CHS. Then H can also be dissected by parallel oblique lines L'_i $(i = 1, 2, \ldots, n)$ so that it decomposes into $n+1$ *oblique zigzag paths* $P'_1, P'_2, \ldots, P'_{n+1}$ such that the one most-left P'_1 and the one most-right P'_{n+1} must be of even length,

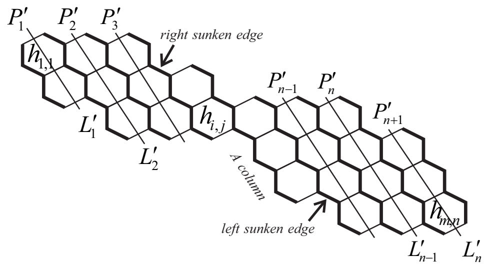


Figure 9. A right monotonic CHS.

and all other paths are of odd length (see Fig. 9). All the hexagons which intersect L'_i $(i = 1, 2, \ldots, n)$ form a linear hexagonal chain, called the i-th *column* of H. In this section, an edge on the left (resp. right) boundary of H is called a *left* (resp. *right*) *sunken edge* if its end vertices both have degree 3. The most-left hexagon $h_{1,1}$ on the top row of H and the most-right hexagon $h_{m,n}$ on the bottom row of H are called the two *corners* of H.

The following theorem can characterize the singular monotonic CHSs.

Theorem 3.1. *Let H be a right monotonic CHS with m rows and n columns except $P(1,1)$ and $P(2,2)$. Then H is singular if and only if it has k pairs of left and right sunken edges $\{e_{1,u}, e_{2,u}\}, u = 1, 2, \ldots, k, k \geq 1$, satisfying the following two conditions (see Fig. 10):*

(1) $e_{1,1}$ lies in P'_2 and not in P_2, $e_{2,1}$ lies in P_2 and not in P'_2; $e_{1,k}$ lies in P_m and not in P'_n, $e_{2,k}$ lies in P'_n and not in P_m;

(2) For $u = 2, 3, \ldots, k$, $e_{1,u}$ and $e_{2,u-1}$ lie in one oblique zigzag path, and $e_{2,u}$ and $e_{1,u-1}$ lie in one horizontal zigzag path.

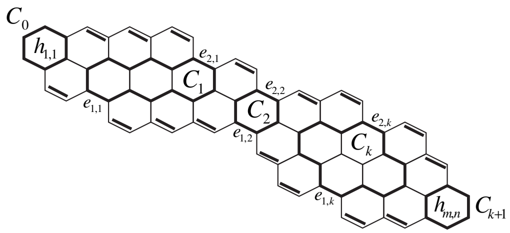


Figure 10. A monotonic CHS satisfying Conditions (1) and (2) of theorem 3.1.

Proof. We first prove the *sufficiency*. Suppose that H has $k \geq 1$ pairs of left and right sunken edges $\{e_{1,u}, e_{2,u}\}$ with Conditions (1) and (2). We can see that $h_{1,1}$ and $h_{m,n}$ each has exactly two inner edges. Let C_0 be $h_{1,1}$, and C_{k+1} be $h_{m,n}$. Let C_j be the boundary of a parallelogram including $e_{1,j}$ and $e_{2,j}$ as the peripheral edges and having the local structure illustrated in Figs. 2(5), 3 and 6 for $j = 1, 2, \ldots, k$. For example, see Fig. 10. Then we can check that the subgraph $\mathcal{C}$ composed of the C_j's, $0 \leq j \leq k+1$, satisfies Conditions (1), (2) and (3) of theorem 2.3, where two disjoint perfect matchings M_1 and M_2 of $\mathcal{C}$ are chosen as follows: For each $0 \leq i \leq k$, if the perfect matching of C_i with the left (resp. right) vertical edges is given to M_1 (resp. M_2), then the perfect matching of C_{i+1} with the right (reps. left) vertical edges is given to M_1 (resp. M_2). Consequently, H is singular.

Next we prove the *necessity*.

Suppose that H is singular. Then H has a subgraph $\mathcal{C}$ consisting of at least one disjoint cycles satisfying Conditions (1), (2) and (3) of theorem 2.3 and each cycle of $\mathcal{C}$ bounds a parallelogram by Lemma 2.7.

Claim 1: P_1 has at least one edge e_0 in $E(\mathcal{C})$.

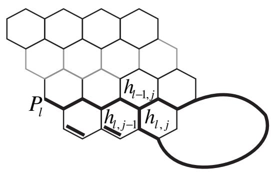


Figure 11. Illustration for the proof of Claim 1.

Let l be the minimum number such that P_l has an edge e in a cycle C of $\mathcal{C}$ (see Fig. 11). If $l \geq 2$, let $h_{l,j}$ be the hexagon on the top left corner of the parallelogram surrounded by C. Then at least one of hexagons $h_{l,j-1}$ and $h_{l-1,j}$ belongs to H. For labellings of hexagons and their edges, we may refer to the last section. If $h_{l,j-1}$ is a hexagon of H, then $e_{bl}(h_{l,j-1})$ is a fixed matching edge relative to $\mathcal{C}$, and $e_{tl}(h_{l,j-1})$ cannot belong to any cycle of $\mathcal{C}$, otherwise P_{l-1} has an edge in $\mathcal{C}$. Therefore all edges of $h_{l,j-1}$ except the one shared with $h_{l,j}$ cannot belong to any cycle of $\mathcal{C}$. Hence $|E_i(h_{l,j-1}) \cap E(\mathcal{C})| = 1$, which contradicts lemma 2.4. If $h_{l-1,j}$ is a hexagon of H and $h_{l,j-1}$ is not a hexagon of H, we can also see that $h_{l-1,j}$ has exactly one edge in $\mathcal{C}$, so $|E_i(h_{l-1,j}) \cap E(\mathcal{C})| = 1$, a contradiction. Hence $l = 1$ and the claim holds.

Claim 2: The hexagon $h_{1,1}$ is one cycle of $\mathcal{C}$.

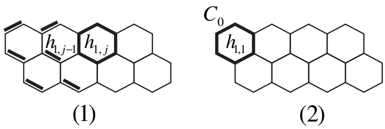


Figure 12. Illustration for the proof of Claim 2.

Let C_0 be the cycle of $\mathcal{C}$ that contains an edge e_0 of P_1. Then C_0 must be a hexagon. Otherwise, C_0 bounds a $P(p, q)$ with p or $q \geq 2$, and C_0 has exactly two peripheral edges of H, which are not adjacent, by Lemmas 2.9 and 2.10, an obvious contradiction. If C_0 is $h_{1,j} (j \geq 2)$, we can see that $|E_i(h_{1,j-1}) \cap E(\mathcal{C})| = 1$, a contradiction to lemma 2.4. Hence, $C_0 = h_{1,1}$ (see Fig. 12).

Claim 3: There is a pair of left and right sunken edges $e_{1,1}$ and $e_{2,1}$ satisfying Condition (1) of this theorem.

We know that $|E_i(h_{1,1}) \cap E(\mathcal{C})|$ is an even number by lemma 2.4, and $h_{1,1}$ has one or two inner edges of H since H has at least two hexagons. So $|E_i(h_{1,1}) \cap E(\mathcal{C})| = 2$, and $h_{1,2}$ and $h_{2,1}$ are two hexagons of H. Applying lemma 2.4 to $h_{1,2}$ and $h_{2,1}$, we find that $e_{br}(h_{1,2})$ and $e_r(h_{2,1})$ must belong to another cycle C_1 of $\mathcal{C}$.

If $C_1 = h_{2,2}$, then neither $h_{1,3}$ nor $h_{3,1}$ is a hexagon of H. Otherwise, $|E_i(h_{1,3}) \cap E(\mathcal{C})| = 1$ by lemma 2.6, or $|E_i(h_{3,1}) \cap E(\mathcal{C})| = 1$ since the other cycles of $\mathcal{C}$ must lie on the right side of C_1 by lemma 2.2, both contradicting lemma 2.4. If $|E_i(h_{2,2}) \cap E(\mathcal{C})| = 2$, then H is $P(2, 2)$, a contradiction. So $|E_i(h_{2,2}) \cap E(\mathcal{C})| = 4$, and $h_{2,3}$ and $h_{3,2}$ are two hexagons of H. In this case, $e_{1,1}$ and $e_{2,1}$ are the first pair of the required sunken edges of H (see Fig. 13).

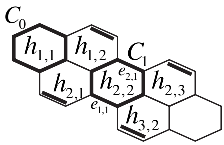


Figure 13. The case that C_1 is a hexagon.

If C_1 bounds a linear chain of at least two hexagons, there are two possibilities by lemma 2.9 as shown in Fig. 14(1) and (2). If C_1 bounds a parallelogram with at least two rows and two columns, there is only one possibility by lemma 2.10 as shown in Fig. 14(3). In any case, let $e_{1,1}$ and $e_{2,1}$ be the peripheral edges of C_1 on the left and right boundary of H respectively. Then $e_{1,1}$ and $e_{2,1}$ satisfy Condition (1) of this theorem. So the claim is verified.

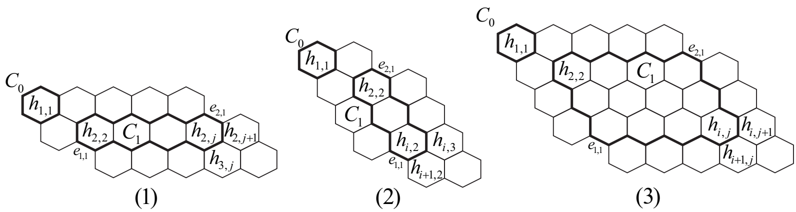


Figure 14. Illustration for C_1 bounding a parallelogram $P(p, q)$ with p or $q \geq 2$.

For short, cycle C_1 in the above three cases always bounds a parallelogram $P(p, q)$ with $p, q \geq 1$, and C_1 has a pair of sunken edges $e_{1,1}$ and $e_{2,1}$.

Let $h_{i,j}$ denote the hexagon on the bottom right corner of the parallelogram bounded by C_1. Then $h_{i+1,j}$ and $h_{i,j+1}$ are two hexagons of H. Applying lemma 2.4 to $h_{i+1,j}$ and $h_{i,j+1}$, we find that $e_{br}(h_{i,j+1})$ and $e_r(h_{i+1,j})$ must belong to one more cycle C_2 of $\mathcal{C}$. So $h_{i+1,j+1}$ is a hexagon of H. If $C_2 = h_{i+1,j+1}$ and $h_{i+1,j+1}$ has exactly two inner edges, then $k = 1$ and the necessity holds. Otherwise, repeating the above process, finally we can obtain a set of pairs of left and right sunken edges $\{e_{1,u}, e_{2,u}\}$ $(u = 1, 2, \ldots, k)$ satisfying the two conditions of this theorem and show that $h_{m,n}$ is a cycle C_{k+1} of $\mathcal{C}$ (see Fig. 10).

■

Remark 3.2. The conditions of theorem 3.1 can have an equivalent description: H has a series of disjoint parallelograms $P(p_0, q_0), P(p_1, q_1), \ldots, P(p_{k+1}, q_{k+1})$ arranged from top to bottom such that the first and the last are hexagons of H on top left corner and bottom right corner respectively, the others have local structures as Fig. 6, and for any consecutive $P(p_i, q_i)$ and $P(p_{i+1}, q_{i+1})$ the bottom right hexagon of $P(p_i, q_i)$ is connected to the top left hexagon of $P(p_{i+1}, q_{i+1})$ by two hexagons. In the sense a single hexagon and $P(2, 2)$ are regarded as satisfying the above conditions as the degenerated cases.

4 General constructable hexagonal system

We now turn to a general CHS H for which a turning row is allowed. We denote by B_i $(i = 1, 2, \ldots, t)$ the i-th turning row of H from top to bottom, and by A_i $(i = 1, 2, \ldots, t{+}1)$ the monotonic CHS consisting of all rows of H sandwiched between B_{i-1} and B_i, where $B_0 = \emptyset$, $B_{t+1} = \emptyset$ and some A_i may be empty for $2 \leq i \leq t$. Moreover, let $\bar{A}_i$ denote the monotonic CHS consisting of A_i and turning rows B_{i-1} and B_i for $i = 1, 2, \ldots, t + 1$. That is, the $\bar{A}_i$ is the maximal monotonic CHS as subgraphs of H, and the consecutive two of them intersect in a turning row. So each $\bar{A}_i$ contains at least two rows of H. For example, the CHS in Fig. 1 has three turning rows with $B_1 = R_3$, $B_2 = R_5$ and $B_3 = R_6$. $A_1 = R_1 \cup R_2$, $A_2 = R_4$, $A_3 = \emptyset$, and $A_4 = R_7$. $\bar{A}_1 = R_1 \cup R_2 \cup R_3$, $\bar{A}_2 = R_3 \cup R_4 \cup R_5$, $\bar{A}_3 = R_5 \cup R_6$, and $\bar{A}_4 = R_6 \cup R_7$.

In this section, we call the most-left (resp. most-right) hexagon on the top row of H when A_1 is right (resp. left) monotonic and the most-right (resp. most-left) hexagon on the bottom row of H when A_{t+1} is right (resp. left) monotonic the two *corners* of H.

Lemma 4.1. *Let H be a CHS with t $(t \geq 1)$ turning rows. If a maximal monotonic CHS $\bar{A}_{t_0}$ $(1 \leq t_0 \leq t+1)$ of H is singular and each corner of $\bar{A}_{t_0}$ has the same two inner edges in H and $\bar{A}_{t_0}$, then H is singular.*

Proof. Suppose that $\bar{A}_{t_0}$ is singular. By theorem 3.1, $\bar{A}_{t_0}$ has a subgraph $\mathcal{C}$ consisting of at least two disjoint cycles as described in remark 3.2 such that the edges of $\mathcal{C}$ can be divided into two matchings M_1 and M_2 satisfying Conditions (1), (2) and (3) of theorem 2.3. We can check that $\mathcal{C}$, M_1 and M_2 also satisfy the same Conditions (1), (2) and (3) for H. First, $M_1 \oplus M_2 = E(\mathcal{C})$ remains. Then, since $\bar{A}_{t_0} - V(\mathcal{C})$ and $H - V(\bar{A}_{t_0})$ each has a perfect matching, $H - V(\mathcal{C})$ has a perfect matching. Moreover, since each corner of $\bar{A}_{t_0}$ has the same two inner edges in H and $\bar{A}_{t_0}$, each hexagon h of H not in $\bar{A}_{t_0}$ has no edges of $\mathcal{C}$, so $AKS_h(M_1) = AKS_h(M_2) = 0$. Hence theorem 2.3 implies that H is singular. ∎

In the following, we introduce two types of connecting two monotonic CHSs, which will paly an essential role in characterizing the singular CHSs.

Type 1: Let A_i be a right monotonic CHS and h_1 be the bottom right corner of A_i, and let A_j be a left monotonic CHS and h_2 be the top right corner of A_j. A_i is connected to A_j by a turning row which has two hexagons h_3 and h_4 each adjacent to both h_1 and h_2 (see Fig. 15(1)).

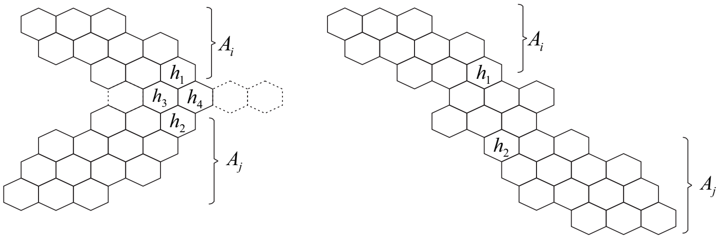


Figure 15. Two types of connecting two monotonic CHSs.

Type 2: Let A_i and A_j be two right monotonic CHSs, and h_1 and h_2 be the bottom right corner of A_i and the top left corner of A_j respectively. A_i is connected to A_j by a left monotonic parallelogram $P(2,3)$ so that A_i is above A_j and h_1 and h_2 each is adjacent to two hexagons of $P(2,3)$ as shown in Fig. 15(2).

Lemma 4.2. *Let a CHS H be obtained by connecting two singular monotonic CHSs A_i and A_j by Type 1 or 2. Then H is singular.*

Proof. By theorem 3.1, A_k $(k = i, j)$ has a subgraph $\mathcal{C}_k$ $(k = i, j)$ consisting of at least two disjoint cycles as described in remark 3.2 satisfying Conditions (1), (2) and (3) of theorem 2.3 for A_k. Then $h_1 \in \mathcal{C}_i$ and $h_2 \in \mathcal{C}_j$.

If A_i and A_j are connected by Type 1, let $\mathcal{C} = \mathcal{C}_i \cup \mathcal{C}_j$. We choose two disjoint perfect matchings M_1 and M_2 of $\mathcal{C}$ as follows: for any pair of consecutive disjoint cycles of $\mathcal{C}$ from top to bottom, if the perfect matching of the upper cycle with the left (resp. right) vertical edges is given to M_1 (resp. M_2), then the perfect matching of the next cycle with the right (reps. left) vertical edges is given to M_1 (resp. M_2). So $M_1 \oplus M_2 = \mathcal{C}$. Obviously, the union of perfect matchings of $A_i - V(\mathcal{C}_i)$ and $A_j - V(\mathcal{C}_j)$ can be extended to a perfect matching of $H - V(\mathcal{C})$. It remains to check all hexagons h in the turning row satisfying (3) of theorem 2.3: $AKS_h(M_1) = AKS_h(M_2) = 0$ or 1 according as h is adjacent to h_1 and h_2 or not. Thus by theorem 2.3 H is singular.

If A_i and A_j are connected by Type 2, let $\mathcal{C}$ consist of the cycles in $\mathcal{C}_1 \cup \mathcal{C}_2$ and the two hexagons on the corners on the connection $P(2,3)$. Note that the two corners have no edges of A_i and A_j. Two disjoint perfect matchings M_1 and M_2 of $\mathcal{C}$ can be chosen by the same rule as the last paragraph. We can check similarly that $\mathcal{C}$, M_1 and M_2 satisfy Conditions (1), (2) and (3) of theorem 2.3 for H. Hence H is also singular. ■

From theorem 3.1 and Lemmas 4.1 and 4.2 we can characterize all singular CHSs: each has a maximal monotonic CHS $\bar{A}_i$ as a singular subgraph so that both corners of $\bar{A}_i$ has exactly two inner edges, only in $\bar{A}_i$, or the subgraph $\bar{A}_i$ is replaced with a series of monotonic singular CHSs connected consecutively by Type 1 or 2. More precisely, we have the following description.

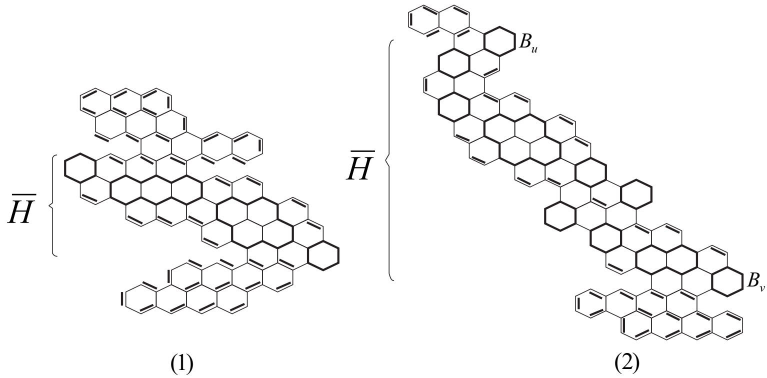


Figure 16. Two examples of singular CHSs.

Theorem 4.3. *Let H be a CHS with t ($t \geq 1$) turning rows. Then H is singular if and only if one of the following two statements holds:*

(1) There is a t_0 ($1 \leq t_0 \leq t+1$) such that $\bar{A}_{t_0}$ of H is singular and each corner of $\bar{A}_{t_0}$ has the same two inner edges in H and $\bar{A}_{t_0}$ (see Fig. 16 (1));

(2) There are u and v ($0 \leq u < v \leq t+1$, $v - u > 1$) such that the subsystem $\overline{H}$ consisting of all rows of H from B_u to B_v satisfies: (a) Each nonempty one of $B_u \cup A_{u+1}$, A_{u+2}, A_{u+3}, ..., A_{v-1} and $A_v \cup B_v$ is singular; (b) Every consecutive pair of nonempty ones in $B_u \cup A_{u+1}$, A_{u+2}, A_{u+3}, ..., A_{v-1} and $A_v \cup B_v$ (empty ones are ignored) are connected

by Type 1 or 2; (c) Each of the two corners of $\overline{H}$ has the same two inner edges in H and $\overline{H}$. (see Fig. 16 (2))

Proof. We first prove the *sufficiency.* If statement (1) holds, then H is singular from lemma 4.1. So suppose that statement (2) holds. For convenience, let $A'_{u+1} = B_u \cup A_{u+1}, A'_i = A_i, u+2 \le i < v$, and $A'_v = A_v \cup B_v$. Then $\overline{H} = \cup_{i=u+1}^{v} A'_i$. By Conditions (a) and (b), if $A'_i \ne \emptyset$, $u+1 \le i \le v$, then A'_i has the subgraph $\mathcal{C}_i$ composed of at least two disjoint cycles as described in remark 3.2. Otherwise, both A'_{i-1} and A'_{i+1} are not empty and connected by Type 2, and let $\mathcal{C}_i$ consist of both corners of the connection $P(2,3)$. Let $\mathcal{C} = \cup_{i=u+1}^{v} \mathcal{C}_i$. In the same method as in the proof of lemma 4.2 we can choose two disjoint perfect matchings M_1 and M_2 of $\mathcal{C}$ and show that they satisfy Conditions (1), (2) and (3) of theorem 2.3 for $\overline{H}$. Hence $\overline{H}$ is singular. Further, since any perfect matching of $\overline{H}$ can extend to a perfect matchings of H and the two corners of $\overline{H}$ has the same two inner edges in $\overline{H}$ and H (Condition (c)), we can check that $\mathcal{C}$, M_1 and M_2 also satisfy Conditions (1), (2) and (3) for H similar to the proof of lemma 4.1. Hence H is singular.

We now prove the *necessity.*

Suppose that H is singular. Then H has a subgraph $\mathcal{C}$ satisfying (1), (2) and (3) of theorem 2.3 and each cycle of $\mathcal{C}$ bounds a parallelogram by Lemma 2.7.

Claim 1: If a cycle C of $\mathcal{C}$ contains some hexagon of a turning row in its interior, then C is an end hexagon of this row and has exactly two inner edges in H.

Suppose to the contrary that C is not a hexagon. Then C bounds a parallelogram which has m rows and n columns with m or $n \ge 2$. By Lemmas 2.9 and 2.10, the local structure of C is as shown in Fig. 17. Let R'_i $(i = 0, 1, \ldots, m+1)$ denote the

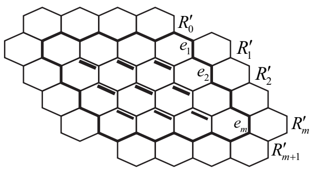


Figure 17. Illustration for the proof of Claim 1.

row of H containing the i-th row of the local structure of C from top to bottom and e_i $(i = 1, 2, \ldots, m)$ the right vertical edge of C in R'_i. Then H has a perfect matching M such that C is M-alternating and all e_i's belong to M. From the local structure of C, we can see that for $2 \le i \le m-1$, e_{i-1} is on the left side of e_i and e_{i+1} is on the right side of

e_i. By lemma 2.2, R_i' $(2 \le i \le m-1)$ turn to right. Furthermore, the two sunken edges make R_1' and R_{m+1}' turn to right. Thus all R_i's $(i = 0, \ldots, m+1)$ form a right monotonic CHS, contradicting some R_i', $1 \le i \le m$, being a turning row. Hence C is a hexagon of the turning row.

Suppose that C is a hexagon of a right turning row. Then C can only be the most-right hexagon of this row. Otherwise, the next hexagon of C on the right-side has only one inner edge in $E(\mathcal{C})$, which contradicts lemma 2.4. On the other hand, the most-right hexagon of the right turning row has at most 3 inner edges. Applying lemma 2.4 to this hexagon, we obtain that this hexagon has exactly two inner edges. So Claim 1 is verified.

Let u be the minimal integer such that $A' = B_u \cup A_{u+1}$ has a hexagon in the interior of a cycle C_0 in $\mathcal{C}$ for $u \ge 0$. Using the same method in Claims 1 and 2 of theorem 3.1, we can show that C_0 must be a hexagon h_{i_0,j_0} of the first row B_u of A'. By Claim 1 this hexagon is an end of B_u, say the *most-left end*, and has exactly two inner edges, which belong to B_u and the next row. So h_{i_0,j_0+1} and h_{i_0+1,j_0} are two hexagons of H.

Claim 2: $\mathcal{C}$ has a cycle C_1 in A' that has some hexagon of the last row of A' in its interior (see Fig. 18).

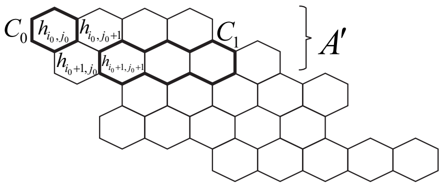


Figure 18. Illustration for the proof of Claim 2.

If C_0 is a hexagon in the last row of A', the Claim holds trivially. Otherwise, A' has at least two rows, and there is another cycle C of $\mathcal{C}$ that contains $e_{br}(h_{i_0,j_0+1})$ and $e_r(h_{i_0+1,j_0})$. By Claim 1, C cannot go through vertical edges of a turning row and is contained in A'. Similar to theorem 3.1, repeating this process, we can find a cycle C_1 of $\mathcal{C}$ in A' that has some hexagon of the last row of A' in its interior. So Claim 2 holds.

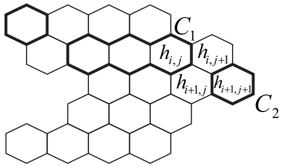


Figure 19. Illustration for the proof of Claim 3.

Claim 3: If C_1 bounds a parallelogram $P(p,q)$ with p or $q \geq 2$ (see Fig. 19), then $\bar{A}_{u+1} = A' \cup B_{u+1}$ satisfies Condition (1) of this theorem.

Let $h_{i,j}$ be the hexagon on the bottom right corner of the parallelogram surrounded by C_1. By the local structure of C_1 we have that $h_{i,j+1}$ and $h_{i+1,j}$ are two hexagons of H and there is another cycle C_2 of $\mathcal{C}$ which contains $e_{br}(h_{i,j+1})$ and $e_r(h_{i+1,j})$. By Claim 1, C_2 can only be the hexagon $h_{i+1,j+1}$, which has exactly two inner edges. By theorem 3.1 $\bar{A}_{u+1}$ is singular and Claim 3 holds.

So, from now on suppose that C_1 is a single hexagon $h_{i,j}$ (for simplicity, let $h_1 = h_{i,j}$). If $|E_i(h_1) \cap E(\mathcal{C})| = 6$, then $|E_i(h_{i-1,j+1}) \cap E(\mathcal{C})| = 1$, contradicting lemma 2.4. If $|E_i(h_1) \cap E(\mathcal{C})| = 2$, then $B_{u+1} = \emptyset$ and $\bar{A}_{u+1} = A'$ is singular and Condition (1) holds. The remaining case is $|E_i(h_1) \cup E(\mathcal{C})| = 4$. By lemma 2.8, there are two possible local structures of h_1 as shown in Fig. 20. If h_1 has the local structure as shown in Fig. 20(1),

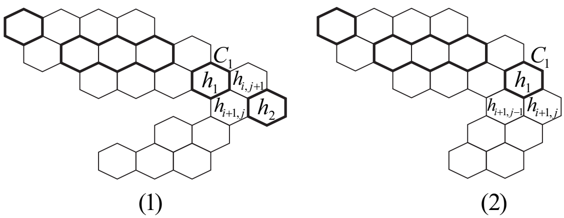


Figure 20. Illustration for the two local structures of h_1.

then $h_{i,j+1}$ and $h_{i+1,j}$ are two hexagons of H. Similarly as Claim 3, $A' \cup B_{u+1}$ is singular and Condition (1) holds.

So suppose that h_1 has the local structure as shown in Fig. 20(2). Similarly we have that $A' = B_u \cup A_{u+1}$ is singular. We now show that Condition (2) happens. There are the following two cases.

Case 1: $A_{u+2} \neq \emptyset$, i.e., there is a row between B_{u+1} and B_{u+2}.

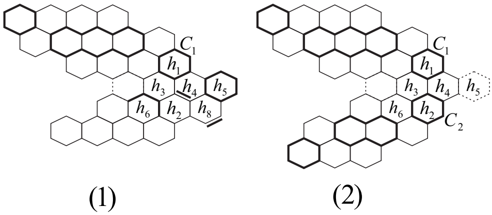


Figure 21. Illustration for Case 1.

Applying lemma 2.4 to $h_3 = h_{i+1,j-1}$, we obtain that one of $e_{bl}(h_3)$ and $e_{br}(h_3)$ belong to a cycle C' of $\mathcal{C}$. If $e_{bl}(h_3)$ belongs to C' (see Fig. 21(1)), then $h_6 = h_{i+2,j-2}$ is a hexagon of H, $e_r(h_6)$ belong to C' and $e_{bl}(h_4)$ is a fixed matching edge relative to $\mathcal{C}$. Applying lemma 2.4 to h_4, we find that $h_5 = h_{i+1,j+1}$ is another cycle of $\mathcal{C}$ with two inner edges by Claim 1 and $h_8 = h_{i+2,j}$ is a hexagon of H. Thus $e_{br}(h_8)$ is a fixed matching edge relative to $\mathcal{C}$ and $|E_i(h_8) \cap E(\mathcal{C})| = 1$, which contradicts lemma 2.4. Hence $e_{br}(h_3)$ belongs to a cycle C_2 of $\mathcal{C}$ (see Fig 21(2)). So $e_{bl}(h_4) \in E(C_2)$, but $e_{br}(h_4) \notin E(C_2)$. Then C_2 bounds a linear chain. If its length is more than one, $e_r(h_2)$ is a sunken edge by lemma 2.9, which contradicts that the next row turns left. So $C_2 = h_2 = h_{i+2,j-1}$. Since h_2 has at least three inner edges, $|E_i(h_2) \cap E(\mathcal{C})| = 4$ or 6. If $e_r(h_2)$ is an inner edge, then h_5 must be a cycle of $\mathcal{C}$ and $|E_i(h_4) \cap E(\mathcal{C})| = 3$, a contradiction. So $|E_i(h_2) \cap E(\mathcal{C})| = 4$, and h_2 has the same local structure with h_1. Hence A' and A_{u+2} are connected by Type 1.

Case 2: $A_{u+2} = \emptyset$, i.e. there is no row between B_{u+1} and B_{u+2} (see Fig. 22).

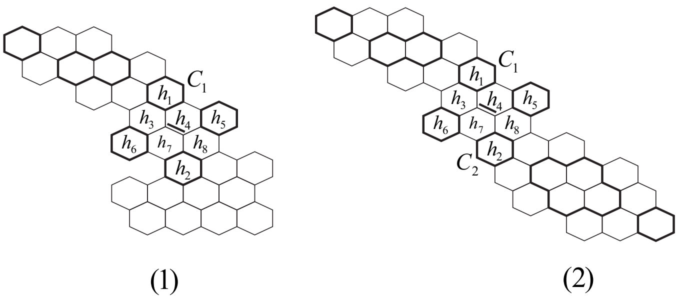


Figure 22. Illustration for Case 2.

Applying lemma 2.4 to $h_3 = h_{i+1,j-1}$, we obtain that $e_{bl}(h_3)$ or $e_{br}(h_3)$ belong to a cycle C'' of $\mathcal{C}$. By Claim 1 C'' must be hexagon h_6, the most-left end of B_{u+2}. Further by lemma 2.8 we obtain that h_6 has exactly two inner edges shared with hexagons h_3 and h_7 of H. Thus $e_{tr}(h_7)$ is a fixed matching edge relative to $\mathcal{C}$. Applying lemma 2.4 to $h_4 = h_{i+1,j}$, we find that $h_5 = h_{i+1,j+1}$ is another cycle of $\mathcal{C}$, the most-right end of B_{u+1}, and $h_8 = h_{i+2,j}$ is a hexagon of H by Claim 1. So A' and A_{u+3} are connected by Type 2. Applying lemma 2.4 to h_7 and h_8, we find that $e_{br}(h_7)$ and $e_{bl}(h_8)$ belong to a cycle C_2 of $\mathcal{C}$. We claim that the row below h_7 and h_8 is not a turning row. Otherwise, the row is a right turning row, and the most-right end belongs to $\mathcal{C}$, a contradiction. Similar to the Case 1, we have that $C_2 = h_2 = h_{i+3,j-1}$ and has the same local structure with h_1.

For short, h_2 is a hexagon of $\mathcal{C}$ lying on one corner of A_{u+2}. Starting this, we continue the above process and finally find the subsystem $\overline{H}$ from the first row of A' to a turning row or the last row of H which satisfies (a), (b) and (c) in Condition (2). ■

As an example, we consider the CHS in Fig. 1. By theorem 3.1 we can check that all $B_{i-1} \cup A_i$'s and $\bar{A}_i$'s $(i = 1, 2, 3, 4)$ of the CHS are nonsingular. So theorem 4.3 implies that this CHS is nonsingular.

5 Applications

In this section, we determine all singular graphs in several typical classes of HS using the characterizations described in the last two sections.

(1) **Parallelogram**

For a benzenoid parallelogram $P(p, q)$ with p or $q \geq 2$, it is known that $P(p, q)$ is singular if and only if $p = q = 2$ from ref. [21]. theorem 3.1 implies obviously this fact.

(2) **Truncated parallelogram**

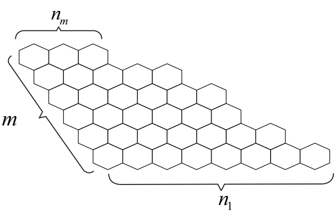
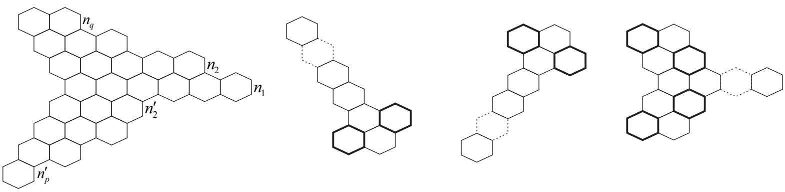


Figure 23. Truncated parallelogram $TP(8, 7, 6, 6, 5, 3)$.

A right monotonic CHS is a *truncated* parallelogram if the most-left hexagons of all rows form a linear hexagonal chain. Let $TP(n_1, n_2, \ldots, n_m)$ be the truncated parallelogram so that the i-th row has n_i hexagons, $i = 1, 2, \ldots, m$, from bottom to top (see Fig. 23). theorem 3.1 implies that $TP(n_1, n_2, \ldots, n_m)$ with at least two hexagons is nonsingular except $P(2, 2)$.

(3) **Truncated chevron**

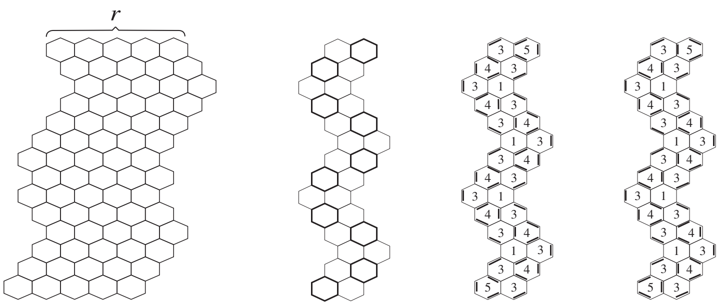


(1) (2) (3) (4)

Figure 24. A truncated chevron and all possible singular truncated chevrons.

We denote by $TC(n'_p, \ldots, n'_2, n_1, n_2, \ldots, n_q)$ the truncated chevron obtained by merging the bottom row of truncated parallelogram $TP(n_1, n_2, \ldots, n_q)$ and the top row of the reflection of another truncated parallelogram $TP(n'_1, n'_2, \ldots, n'_p)$ along a horizontal line where $n'_1 = n_1$ (see Fig. 24(1)). By theorem 4.3 we have that $TC(n'_p, \ldots, n'_2, n_1, n_2, \ldots, n_q)$ is singular if and only if it is isomorphic to $TC(2, 2, 1, \ldots, 1)$, or $TC(2, 2, n_1, 2, 2)$ with $n_1 \geq 2$ (see Fig. 24(2) to (4)).

(4) **Multiple chain**



(1) (2) (3) (4)

Figure 25. An example for $M(5)$, and $M_0(2)$ with the same AKS corresponding to two GKSs.

A multiple chain $M(n)$ is a CHS so that each row has n hexagons and the leftmost hexagons of all rows form a hexagonal chain (see Fig. 25(1)). In particular, let $M_0(2)$ be a multiple chain $M(2)$ so that there are two rows above the first turning row and below the last turning row respectively, and there are two rows between any two consecutive turning rows (see Fig. 25(2)), including the degenerated case $P(2,2)$. By theorem 4.3 we can see that $M(n)$ is singular if and only if it is isomorphic to $M_0(2)$.

6 Concluding remarks

In this paper, we have characterized the constructable hexagonal systems that are singular, which have no one-to-one correspondence between GKS and AKS. As applications we found out all singular graphs in several typical classes of CHSs as parallelograms, truncated parallelograms and chevrons, and multiple chains. Gutman et al. [10] showed that the unique singular graph for cata-condensed HSs is the single hexagon. Such conclusions shows that there are only a small number of singular graphs among them. For further researches, we may consider the following problems:

(1) How to characterize general peri-condensed HSs that are singular? For other typical classes of non-contructable HSs, such as rectangle-, pentagon- and hexagon-shaped benzenoids, etc., (see [6]), find out the singular graphs. Perhaps it is necessary to analyze the local structures of the cycle C of $\mathcal{C}$ described in theorem 2.3 that bounds a hexagon-shaped HS or a concave HS.

(2) Let α and γ denote the numbers of AKS and GKS of an HS H respectively. It is obvious that $\alpha/\gamma = 1$ when H is nonsingular and $0 < \alpha/\gamma < 1$ otherwise. This ratio implies the extent of singularity of an HS. It is necessary to study the accumulation points or the density of the ratios of all HSs with perfect matchings in the interval $(0, 1]$.

(3) For other graphs, such as rotagraphs (closed benzenoid strips), coronoid benzenoids, and fullerene graphs, etc., partition of π-electrons in rings has been considered [2, 3, 8, 9, 11]. Graovac et al. [11] showed that the ratios α/γ within benzo[e]pyrenic rotagraphs can tend towards 0. It is natural to consider one-to-one correspondence between GKS and AKS and the the ratios α/γ for such graphs.

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