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Forcing hexagons in hexagonal systems

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Dedicated to Prof. Fuji Zhang on the occation of his 70th birthday

Abstract

We introduce the concept of a forcing hexagon in a hexagonal system H, which is a hexagon h in H such that the subgraph of H obtained by deleting all vertices of h together with their incident edges has exactly one perfect matching. We show that any hexagonal system with a forcing hexagon is a normal hexagonal system. We further prove that every hexagon of a hexagonal system H is forcing if and only if H is a linear hexagonal chain, and that any other hexagonal system has at most two forcing hexagons. Using the tool of Z-transformation graphs developed by F. Zhang et al, we prove the co-existence property of forcing hexagons and forcing edges, and we obtain the structural characterizations for the hexagonal systems with a given number of forcing hexagons. Miscellaneous related results are presented. We also post a question for further investigation.

1 Introduction

Perfect matchings in hexagonal systems, which coincide with Kekulé patterns in benzenoid hydrocarbons, have long been attracting interests of many chemists as well as graph theorists. Various research has been devoted to this topic (for example, see the books [3], [5] and [6]).

In this paper we will introduce a new concept called forcing hexagons in a hexagonal system. The motivation came from two aspects: one is the well known notion of Clar structures defined by Clar in 1972 (cf. [5]); the other is the concept of forcing edges introduced by F. Harary et al [7] in 1991.

A *Clar structure* of a hexagonal system H is obtained by drawing circles in some hexagons of H and these circles represent the so-called "*aromatic sextets*". The three rules of drawing circles are as follows:

(a) circles are not allowed to be drawn in adjacent hexagons;

(b) circles can be drawn in hexagons if the rest of H either has at least one Kekulé structure or is empty;

(c) a Clar structure contains the maximum number of circles which can be drawn using (a) and (b).

The Clar structures represent the modes of cyclic conjugation of the π-electrons in benzenoid hydrocarbons. The number of *aromatic sextets* in a Clar structure of H is called the Clar number of H and denoted as $C(H)$. It is obvious that the Clar number of any given benzenoid system is unique no matter which circles are drawn. The main chemical implication of the Clar number is the following empirically established regularity: Given two isomeric benzenoid hydrocarbons, the compound with greater Clar number is more stable both chemically and thermodynamically.

The concept of forcing edges is defined as follows. An edge in a hexagonal system H is called a *forcing edge* if it belongs to exactly one perfect matching of H. In 1995, F. Zhang and X. Li [19] obtained characterizations for the hexagonal systems with forcing edges and determined all forcing edges in such systems.

Motivated by the above, we introduce a new concept called forcing hexagons as follows.

Definition 1.1 A hexagon h of a hexagonal system H is called a forcing hexagon of H if $H - h$ has exactly one perfect matching.

Note:

1. $H-h$ is meant to be the subgraph of H obtained by deleting all vertices of h together with their incident edges.

2. If H is the single hexagon h, then h is a forcing hexagon of H. It is because the empty graph $H - h$ is assumed to have exactly one perfect matching by convention.

The following questions naturally arise:

Q1. Does every hexagonal system have a forcing hexagon?

Q2. How many forcing hexagons can a hexagonal system have?

Q3. How to characterize the hexagonal systems with a given number of forcing hexagons?

Q4. Is there any relationship between forcing hexagons and forcing edges of a hexagonal system?

All these questions will be answered in this paper. Moreover, we will give miscellaneous related results and correct an error in an illustrative example in the Appendix of [1]. We will also post a question for further investigation.

2 Preliminaries

A *hexagonal system*, which is also called a polyhex graph and often used to represent a benzenoid hydrocarbon, is a finite 2-connected subgraph of the hexagonal lattice, in which every inner face is a hexagon. Any two hexagons of a hexagonal system either have a common edge or have no common vertices, and we say the two hexagons are *adjacent* (*disjoint*, resp.) in the former (latter, resp.) case.

The *inner dual* of a hexagonal system H is the graph H^* in which each vertex h^* corresponds to the center of a hexagon h of H, and two vertices h_1^* and h_2^* are adjacent in H^* if and only if their corresponding hexagons h_1 and h_2 are adjacent in H. A hexagonal system H is called a *cata-condensed hexagonal system* if its inner dual H^* is a tree. A hexagonal system H is called a *hexagonal chain* if H^* is a path. In particular, H is called a *linear hexagonal chain* if H^* is a straight path.

A *perfect matching* of a graph is a set of pairwise disjoint edges of the graph that cover all its vertices. Let G be a graph with a perfect matching M. Then the edges of G can be divided into two classes: the edges in M are called *M-double bonds*, and the other edges are called *M-single bonds*. They may also be simply called double bonds or single bonds without the prefix M when there is no need to specify the perfect matching involved. An *M-alternating cycle* (resp. *M-alternating path*) of G is a cycle (resp. path) of G whose edges are alternatively in M and $E(G) - M$, where $E(G)$ is the set of edges of G.

For simplicity, we always assume that any hexagonal system H is embedded in the plane with some of its edges vertical. The sets of three circularly arranged double bonds in a hexagon of a perfect matching of H are called *proper sextet* and *improper sextet*, respectively, as indicated in Fig. 1.

Figure 1: Proper sextet (I) and improper sextet (II)

It is clear that an *M-alternating hexagon* of a hexagonal system H may contain either a proper sextet or an improper sextet of H. So, a hexagon h of H is a forcing hexagon if and only if there are exactly two perfect matchings M_i, $i = 1, 2$, such that h is M_i-alternating, i.e., one of the two has a proper sextet on h but the other has an improper sextet on h.

Let $f(H)$ denote the number of forcing hexagons of H. It is obvious that $0 \leq f(H) \leq n$, where n is the number of hexagons of H. The existence of both extreme cases can be easily verified by the examples given in Fig. 2.

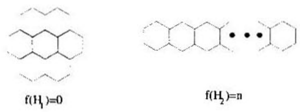


Figure 2: Coronene H_1 and a linear hexagonal chain H_2 with n hexagons

A *generalized hexagonal system* is a graph obtained from a hexagonal system H by deleting all the vertices and edges which lie in the interiors of a group of separated cycles $C_1, C_2, \cdots, C_k$ of H such that no C_i includes another C_j in its interior. So the generalized hexagonal systems contain not only the hexagonal systems but also those changed hexagonal systems with "holes".

It is well known (for example, see [14]) that a hexagonal system has at least two different perfect matchings if it has one. This is also true for generalized hexagonal systems by corollary 2.3 on page 60 in [1].

Lemma 2.1 Let G be a generalized hexagonal system with a perfect matching. Then G has at least two different perfect matchings.

The following lemma in [4] gives a stronger result for hexagonal systems.

Lemma 2.2 For each perfect matching M of a hexagonal system H, there is an M-alternating hexagon in H.

Note that the above lemma can not be extended to the generalized hexagonal systems. For example, the graph G in Fig. 3 is a generalized hexagonal system with n holes and a perfect matching M without M-alternating hexagons.

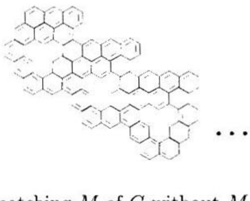


Figure 3: A perfect matching M of G without M-alternating hexagons

Let H be a hexagonal system with perfect matchings. An edge of H is called a *fixed single bond* (resp. *fixed double bond*) if it belongs to no (resp. all) perfect matchings of H. An edge of H is called a *fixed bond* if it is either a fixed single bond or a fixed double bond. H is said to be *normal* if it contains no fixed bonds; *abnormal* otherwise. An abnormal hexagonal system is often called *essentially disconnected* in literature.

In a hexagonal system H with perfect matchings, a maximal connected subgraph which contains no fixed bonds is called a *normal component* of H. It has been proved (cf. [8], [12] or [23]) that any abnormal hexagonal system has at least two normal components, and that every normal component is a normal hexagonal system. So, H is normal if and only if it has exactly one normal component.

There is an inductive representation for the structures of normal hexagonal systems. That is, any normal hexagonal system H with $n > 1$ hexagons can be written as $H = H_{n-1} + h_n$, where H_{n-1} is a normal hexagonal system of $n-1$ hexagons and h_n is a hexagon of H (cf.[8], [9], [21] and [23]). The addition of h_n to H_{n-1} has three possible ways as indicated in Fig. 4.

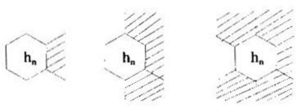


Figure 4: Three possible ways to add h_n to H_{n-1}

To investigate the forcing hexagons of hexagonal systems which are not linear hexagonal chains, we will need the tool of Z-transformation graphs, which was introduced by F. Zhang et al [17]. Let H be a hexagonal system with perfect matchings. The *Z-transformation graph* of H, denoted by $Z(H)$, is the graph whose vertices are the perfect matchings of H where two vertices M_1 and M_2 are adjacent if and only if their symmetric difference $M_1 \oplus M_2$ is a hexagon of H. It should be noted that for a perfect matching M of H, the degree of M in $Z(H)$ is equal to the number of M-alternating hexagons in H.

Lemma 2.3 [18] [19] For any hexagonal system H with perfect matchings, $Z(H)$ is a connected bipartite graph with at most two vertices of degree one.

F. Zhang et al [17] described the structures of hexagonal systems H whose $Z(H)$ has vertices of degree one, by introducing the following coordinate system $O - ABC$ and two related notions.

(I) **Coordinate system O-ABC**

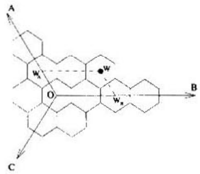


Figure 5: A coordinate system $O - ABC$

Let H be a hexagonal system, s_0 be a hexagon of H, and O be the center of s_0. A *coordinate system* $O - ABC$ with respect to (w.r.t.) s_0 consists of three half-lines originating from O, called axes OA, OB and OC, such that each axis perpendicularly intersects a set of parallel edges of H and the angle between any two axes is 120°, see Fig. 5. The three axes divide the plane into three areas AOB, BOC and COA. For a point W lying in some area, say AOB, let W_A be the intersection point of the axis OA and the line through W and parallel to OB, and let W_B be the intersection point of the axis OB and the line through W and parallel to OA. The coordinates of W, defined to be the lengths of OW_A and OW_B, are denoted by $W(OA)$ and $W(OB)$ respectively.

(II) **Monotone w.r.t. O-ABC**

Let H^* be the inner dual of H. The *perimeter of* H^* is the boundary of its exterior face, i.e., a closed walk in which each cut edge of H^* is traversed twice, see Fig. 6.

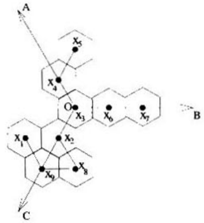


Figure 6: The perimeter of H^* is $x_1x_2x_3x_4x_5x_4x_3x_6x_7x_6x_3x_2x_8x_9x_1$

If the part of the perimeter of H^* lying in some area, say AOB, is a path $W_1W_2\cdots W_t$ after deleting the edges lying on OA and OB, and the path satisfies

$W_1(OA) \geq W_2(OA) \geq \cdots \geq W_t(OA)$ and $W_1(OB) \leq W_2(OB) \leq \cdots W_t(OB)$,

or $W_1(OA) \leq W_2(OA) \leq \cdots \leq W_t(OA)$ and $W_1(OB) \geq W_2(OB) \geq \cdots \geq W_t(OB)$,

then H is said to be monotone in the area AOB. If H is monotone in all three areas, then H is said to be *monotone* w.r.t. the coordinate system $O - ABC$. (Note: Here we use the simpler expression "H is monotone" that has exactly the same meaning as "the perimeter of H^* is monotone" in [18] and [19].)

For example, the hexagonal system in Fig. 7 is monotone w.r.t. O-ABC, but the hexagonal system in Fig. 6 is not.

(III) **3-dividable w.r.t. O-ABC**

A perfect matching M of a hexagonal system H is said to be 3-*dividable* w.r.t. the coordinate system $O - ABC$ provided that any edge of M does not intersect the axes OA, OB and OC, and two edges of M lie in the same area if and only if they are parallel, see Fig. 7.

It should be noted that the hexagon centered at O is the unique M-alternating hexagon in H when M is 3-dividable w.r.t. $O - ABC$.

The following lemma gives two characterizations for the hexagonal systems whose Z-transformation graphs have a vertex of degree one.

Lemma 2.4 [18] For a hexagonal system H, the following statements are equivalent.

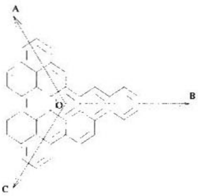


Figure 7: A 3-dividable perfect matching w.r.t. the coordinate system $O - ABC$

(i) $Z(H)$ has a vertex of degree one.

(ii) There exist a hexagon s_0 and a coordinate system $O - ABC$ w.r.t. s_0 and a perfect matching M of H such that M is 3-dividable w.r.t. $O - ABC$.

(iii) There exists a hexagon s_0 and a coordinate system $O - ABC$ w.r.t. s_0 such that H is monotone w.r.t. $O - ABC$.

For hexagonal systems H whose $Z(H)$ has a vertex of degree one, another more intuitive characterization is given in the next lemma, where the notion $S(H)$ denotes the smallest big hexagon that contains the interior of H in its interior and has its edges parallel to the edges of H, see Fig. 8.

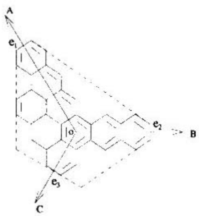


Figure 8: The smallest big hexagon $S(H)$ containing H

Lemma 2.5 [18] Let H be a hexagonal system. Then $Z(H)$ has a vertex of degree one if and only if the following three conditions are satisfied:

(i) There are three pairwise disjoint edges of $S(H)$ each of which contains exactly one edge e_i of H $(i = 1, 2, 3)$.

(ii) The perpendicular bisectors of e_1, e_2 and e_3 intersect at the center O of some hexagon s_0 of H.

(iii) H is monotone w.r.t. the coordinate system $O - ABC$ where the axes OA, OB and OC are the perpendicular bisectors of e_1, e_2 and e_3 respectively, see Fig. 8.

Characterizations of a hexagonal system H with a forcing edge were given by F. Zhang et al [19] in the following lemmas. By a *boundary hexagon* of H we mean a hexagon that has at least one edge on the boundary of H.

Lemma 2.6 [19] Let H be a hexagonal system with perfect matchings. Then H has a forcing edge if and only if $Z(H)$ has a vertex of degree one (or, equivalently, H fulfills the conditions of Lemmas 2.4 and 2.5), and the hexagon s_0 mentioned in Lemmas 2.4 and 2.5 is a boundary hexagon of H.

Lemma 2.7 [19] Let H be a hexagonal system whose $Z(H)$ has exactly two vertices of degree one. Then one of the following three cases must occur.

(i) The perimeter of H^* is a big hexagon and H has no forcing edges, see Fig. 9.

(ii) The perimeter of H^* is a parallelogram with an angle equal to 120° and H has exactly 4 forcing edges, see Fig. 10.

(iii) H^* is a straight path with n vertices and H has $n + 5$ forcing edges, see Fig. 11.

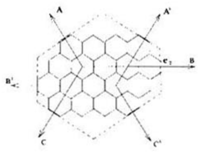
(Note: In Fig. 10 and Fig. 11, all forcing edges are marked by short bars.)

Lemma 2.8 [19] Let H be a hexagonal system whose $Z(H)$ has exactly one vertex of degree one. Then H has at most 3 forcing edges. The three possible forcing edges are the three disjoint edges of s_0 if they lie on the boundary of H, where s_0 is the hexagon mentioned in Lemmas 2.4 and 2.5. See Figures 12, 13 and 14.

(Note: In Fig. 12, Fig. 13 and Fig. 14, all forcing edges are marked by short bars.)

The following result is implied in the proof of Theorem 4 in [18].

Lemma 2.9 Let H be a hexagonal system with perfect matchings. If $Z(H)$ is a path, then for any perfect matching M of degree two in $Z(H)$, H has exactly two M-alternating hexagons and the two hexagons must be adjacent. On the other hand, if there is a perfect matching M of degree two in $Z(H)$ such that H has two adjacent M-alternating hexagons, then $Z(H)$ is a path.



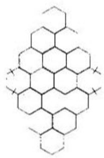


Figure 10: $Z(H)$ has 2 vertices of degree one, H has 2 forcing hexagons and 4 forcing edges

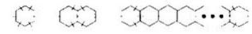


Figure 11: $Z(H)$ has 2 vertices of degree one, H has n forcing hexagons and $n + 5$ forcing edges

The next lemma, which characterizes the hexagonal system H that has $Z(H)$ as a path, was given in [22] as a corollary (Cor. 5.4) of a theorem on plane elementary bipartite graphs. We will provide a more direct proof of the result.

Lemma 2.10 [22] Let H be a hexagonal system. Then $Z(H)$ is a path if and only if H is a linear hexagonal chain.

Our proof will need a result on Clar numbers. Recall that the Clar number $C(H)$ of a hexagonal system H is equal to the maximum number of disjoint M-alternating hexagons, where M runs over all perfect matchings of H. By Lemma 2.2, we immediately see that $C(H) \geq 1$ for any hexagonal system H with a perfect matching. It is natural to consider the extremal case when a hexagonal system has $C(H) = 1$. Such hexagonal systems are characterized in the next lemma (cf. [15], [16] and [17]). Here we will give a different proof using some well known properties of the normal and abnormal hexagonal systems.

Lemma 2.11 A hexagonal system H has $C(H) = 1$ if and only if H is a linear hexagonal chain.

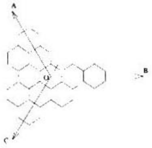


Figure 12: $Z(H)$ has 1 vertex of degree one, H has 1 forcing hexagon and 1 forcing edge

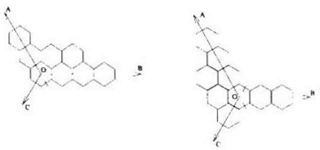


Figure 13: $Z(H)$ has 1 vertex of degree one, H has 1 forcing hexagon and 2 forcing edges

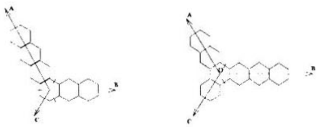


Figure 14: $Z(H)$ has 1 vertex of degree one, H has 1 forcing hexagon and 3 forcing edges

Proof. We only need to show the necessity since the sufficiency is an easy verification.

It is trivial if H has only one hexagon. So we assume that H has $n > 1$ hexagons and $C(H) = 1$. First, we claim that H is normal. Otherwise, H has at least two normal components, each of which is a normal hexagonal system. So $C(H) \geq 2$ because the Clar number is at least one for each normal component of H by Lemma 2.2. It contradicts that $C(H) = 1$. So the above claim is proved.

By the inductive representation for the structures of normal hexagonal systems, H can be decomposed into the form $H = h_1 + h_2 + \cdots + h_n$ such that each h_i is a hexagon of H and $H_i = h_1 + h_2 + \cdots + h_i$ is a normal hexagonal system for all $1 \leq i \leq n$. It is clear that $C(H_j) \geq C(H_i)$ for $n \geq j \geq i \geq 1$. Since $C(H) = 1$, then $C(H_i) \leq 1$ for all i. On the other hand, by Lemma 2.2 we have $C(H_i) \geq 1$ since H_i is a normal hexagonal system for all i. Therefore $C(H_i) = 1$ for all i.

Now it suffices to use the mathematical induction to prove that H_i is a linear hexagonal chain for each i. It is obvious for $i = 1, 2$. Let $i > 2$ and assume that it is true for $i-1$, i.e., H_{i-1} is a linear hexagonal chain. Note that $H_i = H_{i-1} + h_i$. We distinguish two cases for adding h_i to H_{i-1}.

Case 1. The h_i is attached to an end hexagon of H_{i-1} but H_i is not linear hexagonal chain.

Case 2. The h_i is attached to an end hexagon of H_{i-1} so that H_i is a linear hexagonal chain.

In Case 1, we can easily get a perfect matching M of H_i such that H_i has two disjoint M-alternating hexagons: one on h_i and the other on any hexagon which is not adjacent to h_i. This contradicts that $C(H_i) = 1$. So, Case 2 is the only possibility. This shows that $H = H_n$ is a linear hexagonal chain. □

The proof for Lemma 2.10 follows immediately from Lemma 2.9 and Lemma 2.11.

3 Main Results

Theorem 3.1 Every hexagonal system with a forcing hexagon is normal.

Proof. Let H be a hexagonal system with a forcing hexagon h. We prove that H is normal by contradiction. Assume that H is not normal. Then from the known results on essentially disconnected hexagonal systems (cf. [8], [12] or [23]), we see that H must have at least two normal components, each of which is a normal hexagonal system, and that the normal components are the connected components obtained from H by deletion of all fixed double bonds together with their end vertices and of all fixed single bonds without their end vertices. Since h is a forcing hexagon, there is a perfect matching M of H such that h is M-alternating. Hence h does not contain any fixed bonds of H and so h must be in one normal component of H, which is denoted by G_1. Let G_2 be another normal component of H. Obviously, the restriction of M on G_2 is a perfect matching of G_2. Hence by Lemma 2.2, there is an M-alternating hexagon in G_2. It implies that $H - h$ has more than one perfect matching. So, this contradicts that h is a forcing hexagon. □

Theorem 3.1 shows that all abnormal hexagonal systems do not have forcing hexagons, which gives a negative answer to the question Q1. It should also be noted that some normal hexagonal systems do not contain a forcing hexagon either, which can be seen from the example of coronene.

Theorem 3.2 Every hexagon of a hexagonal system H is forcing if and only if H is a linear hexagonal chain.

Proof. The sufficiency can be seen by direct verification. To prove necessity, we first show that $C(H) = 1$ if $f(H) = n$. It is obvious that $C(H) \geq 1$. If $C(H) > 1$, then H has a perfect matching M with at least two disjoint M-alternating hexagons. Clearly, any one of such hexagons is not forcing. This contradicts the hypothesis that $f(H) = n$. So, we must have $C(H) = 1$. Then by Lemma 2.11, H is a linear hexagonal chain. □

By the above theorem, we only need to consider the hexagonal systems that are not linear hexagonal chains.

Theorem 3.3 Let H be a hexagonal system which is not a linear hexagonal chain. Then a hexagon h of H is forcing if and only if

(i) h is a boundary hexagon, and

(ii) there is a perfect matching M of H such that the hexagon h is M-alternating and M has degree one in $Z(H)$.

Proof. First, we prove the necessity.

(i) can be easily seen by contradiction. Otherwise, $H - h$ is a generalized hexagonal system. Since h is forcing, $H - h$ has a unique perfect matching, which contradicts Lemma 2.1.

(ii) can be proved as follows. Since h is forcing, we may let M be a perfect matching of H in which h is an M-alternating hexagon. If M has degree one in $Z(H)$, then it is done. Suppose that the degree of M is at least two in $Z(H)$, then H has at least two M-alternating hexagons. All the M-alternating hexagons different from h must be adjacent to h since h is forcing. Note that the common edge of any two adjacent M-alternating hexagon must be an M-double bond. So h has at most three adjacent hexagons that are also M-alternating hexagons. By Lemma 2.10, $Z(H)$ is not a path since H is not a linear hexagonal chain. It implies that h cannot have exactly one adjacent hexagon that is M-alternating by Lemma 2.9. Therefore, h has either two or three adjacent hexagons that are also M-alternating hexagons. Let $M' = M \oplus h$. Then it is not difficult to check that h is the only M'-alternating hexagon, and so M' has degree one in $Z(H)$. Thus the necessity is proved.

Now we show the sufficiency. Let h be a boundary hexagon of H and let M be a perfect matching of H such that h is M-alternating and M has degree one in $Z(H)$. Let M' be the restriction of M on $H - h$. Obviously, M' is a perfect matching of $H - h$. To show h is forcing, we only need to show that M' is the only perfect matching of $H - h$. This can be proved by contradiction as follows. Assume the contrary and let M'' be another perfect matching of $H - h$. Then $M' \oplus M''$ is a set S of disjoint cycles. Let C be a cycle in S which does not include any other cycle in S. Obviously C is an M'-alternating cycle. Let G denote the subgraph of H that is a hexagonal system with boundary C. Then the restriction of M' on G is a a perfect matching of G. By Lemma 2.2, there is an M'-alternating hexagon h' in G. Obviously h' is also M-alternating. Since h' and h are disjoint M-alternating hexagons in H, it contradicts the condition that M has degree one in $Z(H)$. This completes the proof for sufficiency, and the theorem follows. $\square$

Corollary 3.4 Let H be a hexagonal system which is not a linear hexagonal chain. Then $f(H) \leq 2$, i.e., H has at most two forcing hexagons.

Proof. By Lemma 2.3 and Theorem 3.3. $\square$

Now the question Q2 has been completely answered. To answer the question Q3, we first give the following lemma that provides two characterizations for a hexagonal system, which is not a linear hexagonal chain, having a forcing hexagon.

Lemma 3.5 Let H be a hexagonal system which is not a linear hexagonal chain, and let h be a boundary hexagon of H. Then the following statements are equivalent.

(i) The hexagon h is forcing.

(ii) There exist a coordinate system $O - ABC$ w.r.t. h and a perfect matching M of H such that M is 3-dividable w.r.t. $O - ABC$.

(iii) There exists a coordinate system $O - ABC$ w.r.t. h such that H is monotone w.r.t. $O - ABC$.

Proof. By Lemma 2.4 and Theorem 3.3. $\square$

From Corollary 3.4, we have known that $f(H) = 0$, 1 or 2 for any hexagonal system that is not a linear hexagonal chain. Characterizations for the three possible cases are given below.

Theorem 3.6 Let H be a hexagonal system which is not a linear hexagonal chain. Then

(1) if the perimeter of the inner dual H^* is a parallelogram, then $f(H) = 2$ and the center of a forcing hexagon is located at the vertex of an obtuse angel of the parallelogram.

(2) if there exists a unique coordinate system $O - ABC$ where O is the center of a boundary hexagon h such that H is monotone w.r.t. $O - ABC$, then $f(H) = 1$ and h is the unique forcing hexagon.

(3) $f(H) = 0$ otherwise.

Proof. By Lemmas 2.4, 2.7, 3.5 and Theorem 3.3. □

From Theorem 3.6, we can immediately get the following characterization for the cata-condensed hexagonal system which is not a linear hexagonal chain.

Corollary 3.7 Let H be a cata-condensed hexagonal system which is not a linear hexagonal chain. Then $f(H) \leq 1$ and one of the following two cases must occur.

(1) $f(H) = 1$ if and only if the inner dual H^* is a path of the L-shape, or a star-like tree of the Y-shape, see Fig. 14.

(2) $f(H) = 0$ otherwise.

By Lemma 2.5 and Theorem 3.3, we can obtain a more intuitive characterization for hexagonal systems with forcing hexagons which are not linear hexagonal chains.

Theorem 3.8 Let H be a hexagonal system which is not a linear hexagonal chain, and let h be a boundary hexagon of H. Then h is forcing if and only if the following three conditions are satisfied:

(i) There are three pairwise disjoint edges of $S(H)$ each of which contains exactly an edge e_i of H $(i = 1, 2, 3)$.

(ii) The perpendicular bisectors of e_1, e_2 and e_3 intersect at the center of the hexagon h of H.

(iii) H is monotone w.r.t. the coordinate system $O - ABC$ where O is the center of the hexagon h and the axes OA, OB, OC all start at O and direct to e_1, e_2 and e_3 as their perpendicular bisectors respectively.

By Theorem 3.3 and Corollary 3.4, we can see that to further investigate the hexagonal systems with forcing hexagons as well as the relationship between the forcing hexagons and the forcing edges of a given hexagonal system, we only need to consider those hexagonal systems H whose $Z(H)$ has one or two vertices of degree one. Then by Lemmas 2.7 and 2.8, we immediately get the following two lemmas.

Lemma 3.9 Let H be a hexagonal system whose $Z(H)$ has exactly two vertices of degree one. Then one of the following three cases must occur.

(i) The periphery of H^* is a big hexagon and H has neither forcing hexagons nor forcing edges, see Fig. 9.

(ii) The periphery of H^* is a parallelogram and H has two forcing hexagons and four forcing edges. Furthermore, each forcing hexagon contains exactly two forcing edges, see Fig. 10.

(iii) H^* is a straight path and each hexagon of H is forcing. Furthermore, if h is the unique hexagon of H, then each edge of h is a forcing edge; otherwise, each ending hexagon contains four forcing edges, and any other hexagon has the two vertical edges as forcing edges, see Fig. 11.

Lemma 3.10 Let H be a hexagonal system whose $Z(H)$ has exactly one vertex of degree one. Then H has at most one forcing hexagon h, which is a boundary hexagon such that there exists a coordinate system $O - ABC$ w.r.t. h and H is monotone w.r.t. $O - ABC$. Furthermore, H has at most three forcing edges, which belong to h and are disjoint edges on the boundary of H, see Figures 12, 13 and 14.

Now we can answer the question Q4 as follows.

Theorem 3.11 A hexagonal system has a forcing hexagon if and only if it has a forcing edge. Furthermore, a hexagon h in a hexagonal system is forcing if and only if h contains a forcing edge.

Proof. By Theorem 3.3, and Lemmas 2.3, 2.6, 3.9 and 3.10. □

4 Miscellaneous

A generalized hexagonal system in which each edge belongs to some hexagon is called a generalized polyhex graph in [1]. Let $k_1, k_2, \cdots, k_t$ be the Kekulé patterns of a given generalized polyhex graph G. The *sextet rotation* R is a simultaneous rotation of all the proper sextets of a given Kekulé pattern k_i of G into the improper sextets to give another Kekulé pattern k_j of G, and it is denoted by $R(k_i) = k_j$. The *sextet rotation graph* $D(G)$ of G is a digraph whose vertices are the Kekulé patterns of G and there is a directed edge from k_i to k_j whenever $R(k_i) = k_j$. Any Kekulé pattern of G without proper sextets is called a *root Kekulé pattern* of G. The following theorem was given in [2] for the directed tree structure of the sextet rotation graph of a polyhex graph.

Theorem A Let H be any polyhex graph with Kekulé patterns. Then $D(H)$ is a directed tree and the root of $D(H)$ corresponds to the root Kekulé pattern of H.

By lemma 2.1, the above theorem can have a somewhat stronger form as follows.

Theorem A′ Let H be any polyhex graph with Kekulé patterns. Then $D(H)$ is a non-trivial directed tree and the root of $D(H)$ corresponds to the root Kekulé pattern of H.

It was remarked in [2] that if G is a generalized polyhex graph but not a polyhex graph, then $D(G)$ is a directed k-tree (i.e., the union of k vertex disjoint directed trees) so that G has k root Kekulé patterns, where $k > 1$ or $k = 1$. In Fig. 2 of [2] the examples G_1 and G_2 were given to illustrate that both cases $k > 1$ and $k = 1$ are possible. We found that the example G_2 chosen in Fig. 2 of [2] for the case $k = 1$ is not correct, since G_2 has more than one root Kekulé pattern, as shown in Fig. 15.

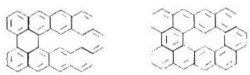


Figure 15: Two root Kekulé patterns of the example G_2 given in [2]

Here we give an infinite class of examples for the case $k = 1$ in Fig. 16. It is not difficult to verify that for each $n \geq 1$, the given generalized polyhex graph with n "holes" has a unique root Kekulé pattern.

5 A Question

It is well known that the concept of forcing edges is related to both chemical and physical problems [10, 11, 13, 20]. For example, let K_{rs} denote the number of Kekulé structures of a benzenoid hydrocarbon in which there is a double bond between the carbon atoms r and

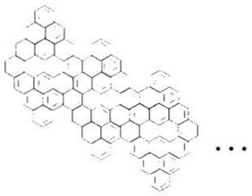


Figure 16: A generalized polyhex graph with n holes and a unique root Kekulé pattern

s, and let K be the total number of Kekulé structures of the benzenoid hydrocarbon. The ratio $P_{rs} = \frac{K_{rs}}{K}$, called the Pauling bond order P_{rs}, is a measure of the order of the chemical bond between the atoms r and s. So, the bond between the carbon atoms r and s in a benzenoid hydrocarbon H is a forcing bond if and only if the Pauling bond order P_{rs} reaches the minimum of all positive Pauling bond orders between carbon atoms of H.

We have revealed in Theorem 3.11 the close relationship between the forcing hexagons and the forcing edges of a hexagonal system. So the concept of forcing hexagons should be related to some chemical and physical properties of benzenoid hydrocarbons. However, for different benzenoid systems, the number of the forcing edges contained in a forcing hexagon may vary between 1,2,3,4 and 6. So we think the following question should be of interest:

Which particular chemical and physical properties of benzenoid hydrocarbons are determined by the (number of) forcing hexagons in their molecular structures?

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