

HEXAGONAL SYSTEMS WITHOUT FIXED DOUBLE BONDS

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ABSTRACT: This note gives a construction method for those hexagonal systems which may only have fixed single bonds but never have fixed double bonds.

1. Notation and Definitions.

A hexagonal system is defined as usual [1]. Let M be a perfect matching of a hexagonal system H . An M -alternating cycle is a cycle whose edges are alternately in M and $E(H)-M$, where $E(H)$ denotes the edge set of H . An edge e of H is called an M -double bond if e belongs to M , otherwise an M -single bond. If e is an M -double bond for any perfect matching M , e is called a fixed double bond. Similarly, if e is an M -single bond for any perfect matching M , e is called a fixed single bond. Since the edges adjacent with a fixed double bond must be fixed single bonds, if H has a fixed double bond it must have a fixed single bond. But the reverse is not true, for example, Prolate rectangle [1] hexagonal system.

For the definitions of cut, p -cut and 2-cut segment, one can find them in ref. [2], [3] and [4] respectively.

In the following, we always assume that H is a hexagonal system with at least one perfect matching. Let C be a cut or g -cut or z -cut segment of H . Then, the graph obtained from H by deleting all the edges intersected by C has exactly two components. If both the two components have perfect matchings, we say that C has property (*).

11. Some Basic Theorems.

For convenience, we always place a hexagonal system in such a manner that its every hexagon has two edges parallel to the vertical line. The following theorem gives a description for those hexagonal systems which may only have fixed single bonds.

Theorem 1: Let H be a hexagonal system. Then, H has no fixed double bonds iff, of the three types of cut segments, H may only have cut segment with property (*).

Proof: If H has g -cut or z -cut segment with property (*), H must have fixed double bonds. Thus, if H has no fixed double bonds, H may only have cut segment with property (*).

Conversely, we wish to prove that, of the three types of cut segments, if H may only have cut segment with property (*), H does not have fixed double bonds. Otherwise, H has a fixed double bond. Then, by lemma 2 of ref.(5), there must be a fixed double bond lying on the contour of H . Suppose e is such a fixed double bond of H . Let the edges e_1, \dots, e_r, e_{r+1} and a hexagon s_0 be shown as in Fig.1, where e_1, \dots, e_r are fixed double bond, e_{r+1}

is not a fixed double bond and s_0 does not belong to H . Let hexagons s, s_1, s_2, s_3 be also shown as in Fig.1.

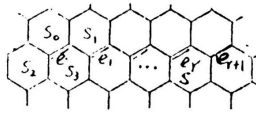
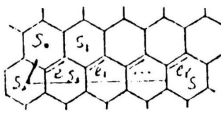
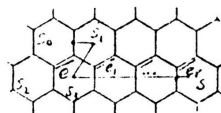


Fig.1

Case 1: The hexagon s does not belong to H . If s_2 belongs to H , a μ -cut segment with property (*) can be found. Otherwise, s_3 must belong to H since s_0 does not belong to H . If s_1 belongs to H , a λ -cut segment with property (*) can be found. Otherwise, a μ -cut segment with property (*) can be found. All of the above bring about contradictions with the hypothesis that H may only have cut segment with property (*). (see Fig.2).



s_2 belongs to H .



s_2 does not belong to H . s_1 belongs to H .



both s_2 and s_1 do not belong to H .

Fig.2

Case 2: The hexagon s belongs to H . Let hexagon s_1 and edges f_1, f_2, \dots be as shown in Fig.3.

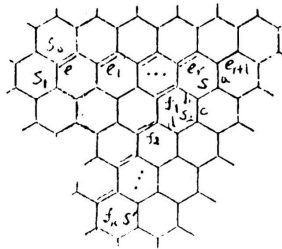
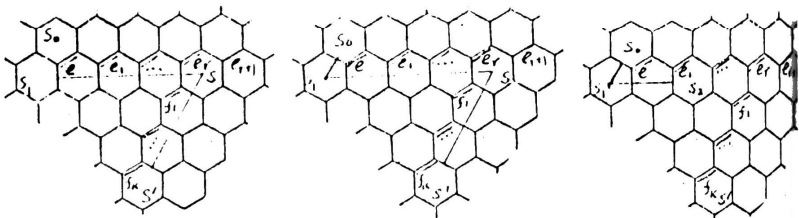


Fig.3

By lemma 1 of ref. [5], one of the edges a and b shown in Fig. 3 must be a fixed single bond of Π . If a is fixed, e_{r+1} must be fixed double bond, a contradiction. Thus b is a fixed single bond. This implies that f_1 is a fixed double bond of Π . Let hexagon s_2 and edges c and d be also shown in Fig. 3. If s_2 does not belong to Π , f_1 is on the contour of Π . Otherwise, one of c and d must be a fixed single bond (again by lemma 1 of ref. [5]). If c is fixed, the edge of s adjacent with both a and b must be fixed double bond since b is a fixed single bond. This implies that e_{r+1} is a fixed double bond, again a contradiction. Continue the above process. At last we arrive at an edge f_k which is a fixed double bond lying on the contour of Π and a hexagon s' which does not belong to Π (see Fig. 5). If s_1 does not belong to Π , a g -cut segment with property (*) can be found. Otherwise, a z -cut or g -cut segment with property (*) can be found. Again, all of the above bring about contradictions with the hypothesis that Π may only have cut segment with property (*). (see Fig. 4).



s_1 does not belong to Π .

s_1 belongs to Π .

s_1 belongs to Π . But some s_2 does not.

Fig. 4

Up to now, our proof is complete.

Theorem 2: Let H be a hexagonal system without fixed double bonds. Then, an edge e of H is a fixed single bond iff H has a cut segment with property $(*)$ such that e is intersected by the cut segment.

Proof: Obviously, if H has a cut segment with property $(*)$ such that e is intersected by the cut segment, e must be a fixed single bond. Conversely, since e is a fixed single bond, by theorem 4 of ref. [4] we know that H has a cut or g -cut or z -cut segment with property $(*)$ intersecting e . By the theorem 1, H must have a cut segment with property $(*)$ intersecting e since H has no fixed double bonds and therefore no g -cut and z -cut with property $(*)$.

Bearing in mind that a non-fixed bond (neither fixed double nor fixed single) of H must be on an M -alternating cycle of H , where M is a perfect matching of H . We have that

Theorem 3: Let H be a hexagonal system, C be a cut or g -cut or z -cut segment of H with property $(*)$. Denote by H_1 and H_2 the two components of the graph obtained from H by deleting all the edges intersected by C . Then, a fixed single (double) bond of H_1 (H_2) must be a fixed single (double) bond of H .

Proof: Obvious.

Theorem 4: Let H be a hexagonal system without fixed double bonds, C and C' be two cut segments of H with property $(*)$. Then, if C is not parallel to C' , the hexagon whose center is the cross

of C and C' must do not belong to H .

Proof: Otherwise, we can find a g -cut segment of H with property (*). Hence, H has a fixed double bond, a contradiction.

III. Construction Method For Hexagonal Systems Without Fixed Double Bonds.

Recall that a normal hexagonal system is a hexagonal system whose each edge is a non-fixed bond. In other words, its every edge is on an M -alternating cycle of it, where M is a perfect matching of it. The term, "normal" is from ref.[1]

Our construction method is based on the construction method for normal hexagonal systems given in ref.[6].

CONSTRUCTION METHOD:

1. If H has no fixed bonds, that is, H is a normal hexagonal system, we can use the method given in ref.[6] to construct it.

2. If H has only fixed single bonds, we use the following induction method to build it up. The fundamental elements are normal hexagonal systems. Suppose that we have built up all the hexagonal systems with n normal subhexagonal systems. For $n+1$, we take one normal hexagonal system H_{n+1} and one built up hexagonal system H with exactly n normal subhexagonal systems H_1, H_2, \dots, H_n . For any orientation of H , join some valleys on the bottom of H_{n+1} with some peaks on the top of H such that no overlapping occurs and the joined peaks of H are only on one of H_1, H_2, \dots and H_n . Then the resultant hexagonal system H^* has only fixed single bonds and $n+1$ subhexagonal systems H_1, \dots, H_n, H_{n+1} .

Fig.5 is an example to demonstrate our construction method, where $n=3$ and $H_{n+1} = H_4$. The vertical heavy edges are newly added.

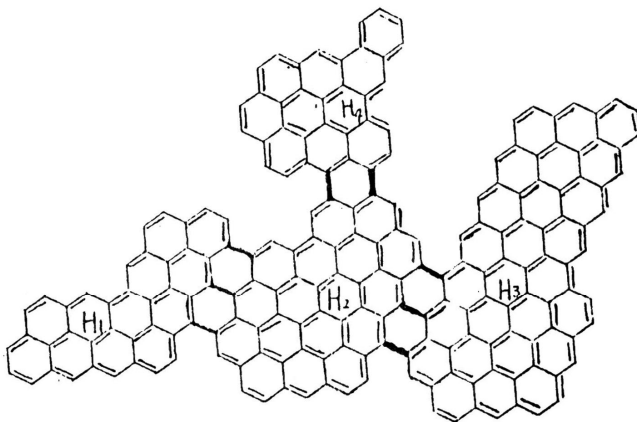


Fig.5

Theorem 4: The hexagonal systems constructed by our CONSTRUCTION METHOD have not fixed double bonds. On the other hand, any hexagonal systems with our fixed double bonds can be constructed by our CONSTRUCTION METHOD.

Proof: The former part is obvious and all the edges connecting two normal subhexagonal systems are fixed single bonds.

Now we prove the latter part. Suppose H is a hexagonal system without fixed double bonds. If H does not have fixed single bonds, step 1 can be used to build up it. Otherwise, by theorem 1 H only has cut segment with property (*). By theorems 3 and 4, there must exist a cut segment C with property (*) such that one of the two components of the graph obtained from H by deleting all the edges

intersected by C is a normal subhexagonal system of H , denoted by H' , and the other is a subhexagonal system of H with at least one perfect matching, denoted by $H-H'$. By theorem 3, $H-H'$ does not have fixed double bonds. In the following, we only need to show that H' has vertices joined to only one normal subhexagonal system of $H-H'$. Otherwise, let H_1 and H_2 be two normal subhexagonal systems of $H-H'$ which have vertices joined to some vertices of H' . Place H in such a manner that the cut segment C is orthogonal to the vertical line. Clearly, there exist a fixed single bond e of $H-H'$ between H_1 and H_2 . By theorem 3, e is also a fixed single bond of H . From theorem 2, H must have a cut segment C' with property (*) intersecting e , and H_1 and H_2 are in different components of the graph obtained from H by deleting all the edges intersected by C' (see Fig.6). Then, C must not be parallel to C' . Since H does not have holes, the hexagon whose center is the cross of C and C' must belong to H . By theorem 4, we get a contradiction with the hypothesis that H does not have fixed double bonds. Since $H-H'$ does also not have fixed double bonds and has less number of normal subhexagonal systems than that of H , by induction we know that our conclusion is true.

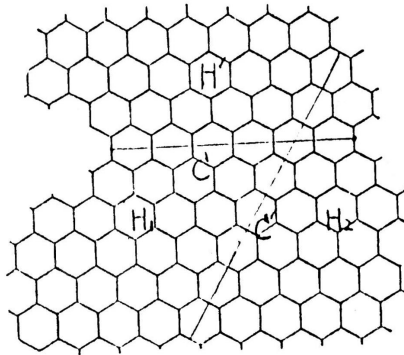


Fig.6

Remark 1: Let H be a HS with at least one perfect matching. We contract every normal subhexagonal system of H into a vertex, and two normal subhexagonal systems are joined with an edge iff there are some edges between them. Then, it is not difficult to see that H has not fixed double bonds iff so defined graph from H is a tree.

Remark 2: Though here we give a construction method for those hexagonal systems which do not have any fixed double bonds, it seems difficult for us to give a simple construction method for hexagonal systems with fixed double bonds.

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