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A FAST ALGORITHM TO DETERMINE FIXED BONDS IN HEXAGONAL SYSTEMS

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ABSTRACT: This paper gives a fast algorithm to determine fixed bonds in a hexagonal system. Consequentially, we can use this algorithm to decompose a given hexagonal system into a number of regions consisting of fixed bonds and a number of normal subhexagonal systems. This decomposition can be used to simplify the procedure of finding Clar formula and counting the number of Kekulé structures for a hexagonal system with fixed bonds.

1. Some Notations and Terminologies.

A hexagonal system (or simply HS) H, also called "hexanimal" or "honeycomb", is a finite 2-connected plane graph in which every interior region is bounded by a regular hexagon of side length 1. Graphs of this kind are of chemical significance since a HS with at least one perfect matching is the skeleton of a benzenoid hydrocarbon molecule. Recall that a perfect matching of a graph G is a set of disjoint edges of G covering all the vertices of G, which coincides with the concept of a Kekulé structure in organic chemistry[1] .

Let M be a perfect matching of a HS H. An M-alternating cycle is a cycle whose edges are alternately in M and E(H)-M, where E(H) is the edge set of H. Let e be an edge of H. If e is contained in M, e is called an M-double bond. Otherwise, e is called an M-single bond. If e is an M -double bond for any perfect matching M_i of H, e is called a fixed double bond. Similarly, if e is an M_i-single bond for any perfect matching M_i of H, e is called a fixed single bond. Both fixed double bonds and fixed single bonds are called fixed bonds. It is not difficult to see that if H contains a fixed double bond, it must contain a fixed single bond. But the reverse is not true.

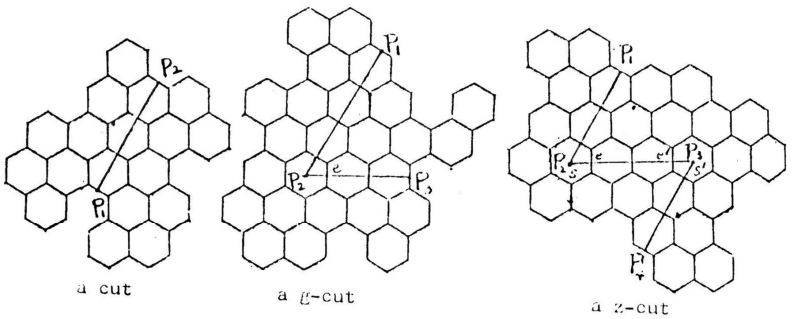
Now we give the definitions for three types of cuts.

Definition 1: A straight line segment $C=P_1P_2$ is called a cut segment of a HS H if

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

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

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



a cut a g-cut a z-cut

Fig.1

Definition 2: A broken line segment $C=P_1P_2P_3$ is called a g-cut segment of a HS H if

(a) P_2 is the center of a hexagon s of H and each of P_1 and P_3 is the center of an edge of H lying on the contour of H;

(b) P_1P_2 is orthogonal to an edge e of s, and P_2P_3 is orthogonal to another edge of s which is adjacent with e;

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

Definition 3: A broken line segment $C=P_1P_2P_3P_4$ is called a z-cut segment of a HS H if

(a) P_2 is the center of a hexagon s of H, P_3 is the center of another hexagon s' of H and P_2P_3 is orthogonal to an edge e of s. Thus, P_2P_3 orthogonally intersects an edge e' of s';

(b) each of P_1 and P_4 is the center of an edge lying on the contour of H, P_1P_2 is orthogonal to an edge of s which is adjacent with e and P_3P_4 is both parallel to P_1P_2 and orthogonal to an edge of s' which is adjacent with e';

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

Fig.1 shows all the three types of cuts, where the former two types of cuts are from ref. [2] and the latter is a new one.

A cut or g-cut or z-cut segment C of a HS H is said to have property (*) if both the two components of the graph obtained from H by deleting all the edges intersected by C have perfect matchings.

In the following, we always assume that H is a HS with at least one perfect matching.

II. Some Basic Theorems.

In order to simplify the discussion, we always place a HS H on the plane so that two edges of its each hexagon are parallel to the vertical line. A vertex of H is called a peak (valley) if it is on the contour of H and above (below) the vertices adjacent to it.

Theorem 1: Let H be a HS. If a cut or g-cut or z-cut segment C of H has property (*), then all the edges intersected by C are fixed single bonds of H.

Proof: Let M be a perfect matching of H. Denote by E(C) the set of edges of H intersected by C, and by H_1 and H_2 the two components of the graph obtained from H by deleting all the edges in E(C). Let J= E(C)∩ M and |J|=k. Now, colour the vertices of H with black and white. Thus, there are exactly k black vertices in H_1 or H_2, say H_1, which are matched with k white vertices in H_2. In other words, the number of black vertices in H_1 is larger than the number of white vertices in H_1 by exactly k, while the number of white vertices in H_2 is larger than the number of black vertices in H_2 by exactly k. Therefore, in any perfect matching of H there must be exactly k black vertices in H_1 matched with k white vertices in H_2. Consequentially, k is independent of the choice of the

perfect matching M. Because C has property (*), H has a perfect matching M' such that for M' the set J is empty, and hence for any perfect matching the set J is empty. That is to say that all the edges intersected by C are fixed single bonds.

Theorem 2: Let H be a HS, C be a cut or g-cut or z-cut segment of H. If one of the two components of the graph obtained from H by deleting all the edges intersected by C has the property that the number of its peaks equals the number of its valleys, then C must have property (*).

Proof: Otherwise, though H has a perfect matching M, both the two components do not have any perfect matching. Therefore, there is at least one edge intersected by C is an M-double bond since the end vertices of the edges intersected by C in one component have the same colour. Thus, the numbers of vertices with different colours in one component do not equal. In other words, in one component the number of peaks is not equal to the number of valleys, a contradiction.

Theorem 3: Let H be a HS. Then for each fixed single bond e of H, there exist a cut or g-cut or z-cut segment with property (*) such that it intersects e.

Proof: We distinguish the following two cases.

Case 1: there is a perfect matching M of H such that the two vertices of e are saturated by two M-double bonds e_1 and e_1' which are not parallel to each other. By the proof of theorem 4 in ref.[2], we know that there exist a cut or g-cut C with property

(*) and intersecting the fixed single bond e.

Case 2: for any perfect matching H of H, the two vertices of e are saturated by two H-double bonds e_1 and e'_1 such that e_1 is parallel to e'_1. Again, by the proof of theorem 4 in ref.[2], we know that e_1 and e'_1 must be fixed double bonds of H. Let $e;e_1,\ldots,e_r,e_{r+1};e'_1,\ldots,e'_l,e'_{l+1}$ be as shown in Fig.2, where $e_1,\ldots,e_r$ and $e'_1,\ldots,e'_l$ are fixed double bonds, but e_{r+1},e'_{l+1} are not.Let $f_2,\ldots,f_p,f_{p+1};f'_2,\ldots,f'_q,f'_{q+1}$ be also as shown in Fig.2, where $f_2,\ldots,f_p;f'_2,\ldots,f'_q$ are fixed double bonds, but f_{p+1},f'_{q+1} are not. Since e_{r+1} and e'_{l+1} are not fixed double bonds, $p\leq r$ and $q\leq l$. Let hexagons s and s' be as shown in Fig.2.

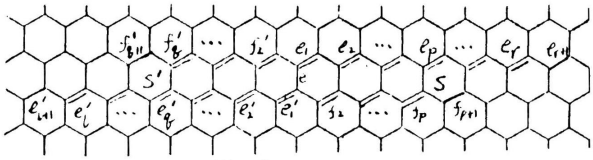


Fig.2

Subcase 2.1: both s and s' do not belong to H. It is obvious that there is a cut segment with property (*) and intersecting e.

Subcase 2.2: one of s and s', say s, belongs to H. Thus, s' does not belong to H. Let the edges $f;g_1,g_2,\ldots;g'_1,g'_2,\ldots,$ and hexagon s_1 be shown as in Fig.3.

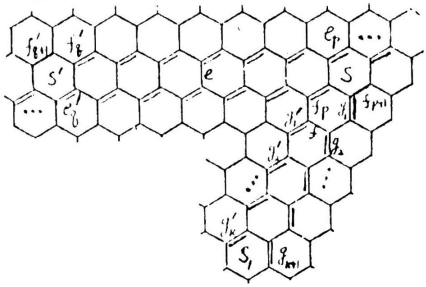


Fig.3

Because f_{p+1} is not a fixed double bond, there must exist a perfect matching M such that g_1 is an M-double bond. Since f_p is a fixed double bond, g'_1 and g_2 must be M-double bonds. Otherwise, f is an M-double bond, and therefore f_p is on an M-alternating cycle, a contradiction. Similarly, we can deduce that $g_3,\ldots,g_{k+1};g'_2,\ldots,g'_k$ are M-double bonds and s_1 is not a hexagon of H. Thus, a g-cut segment with property (*) and intersecting e has been found.

Subcase 2.3: neither s nor s' belong to H. Using the same method as in subcase 2.2 for the two end hexagons s and s', we can find a z-cut segment with property (*) and intersecting the fixed single bond e. Our proof is now complete.

Remark: There indeed exist fixed single bonds which are not intersected by any cut or g-cut segments with property (*). They must be intersected by z-cut segments with property (*). See the following Fig.4, where $e_1,e_2,\ldots,e_m$ are such fixed single bonds.

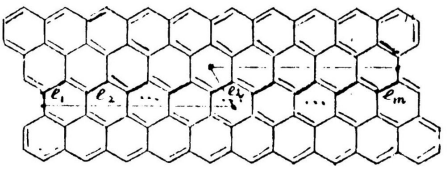


Fig.4

By theorems 1 and 3, we can immediately get the following theorem.

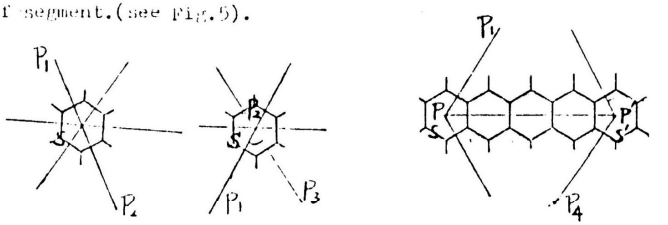
Theorem 4: Let H be a HS. Then an edge e of H is a fixed single bond iff there is a cut or g-cut or z-cut segment with property (*) such that e is intersected by it.

III. A Fast Algorithm for Determining Fixed Bonds in a HS.

Let H be a HS with perfect matchings.

Step 1: From the center of each hexagon s of H, draw all the

3 cut segments and the 6 g-cut segments. For each two hexagons s and s' of H, if the line segment obtained by connecting the two centers P and P' of s and s' is orthogonal to an edge of s, then draw all the two z-cut segments with PP' being one piece of segment.(see Fig.5).



3 cuts 6 g-cuts 2 z-cuts

Fig.5

Step 2: For each such cut or g-cut or z-cut segment, count the number of peaks and the number of valleys in one of the two components of the graph obtained from H by deleting all the edges intersected by that cut.

Step 3: If the two numbers in step 2 are equal for a cut or g-cut or z-cut C, then colour all the edges intersected by C with red. Otherwise, leave them black.

Theorem 5: Let H be a HS. Apply our algorithm to H. Then H is decomposed into a number of independent edges with red colour or black colour and a number of regions consisting of black edges. We assert that

(1) the independent edges with red colour are all fixed single bonds of H;

(2) the independent edges with black colour are all fixed double bonds of H;

(3) the regions consisting of black edges are all normal subhexagonal systems of H, where normal HS means that the HS does not have any fixed bonds. In other words, its every edge is on an M-alternating cycle, where M is a perfect matching of the HS. The term, "normal" is from ref.[1].

Proof: From theorem 3, we know that for each fixed single bond e of H there exist a cut or g-cut or z-cut segment C of H with property (*) such that e is intersected by C.In addition, from theorem 2 we know that by our algorithm we have found out all the cut and g-cut and z-cut segments with property (*). Thus, from theorem 1 we know that all the fixed single bonds of H, if any, must be coloured with red. Obviously,these fixed single bonds are independent of one another. Deleting all the fixed single bonds, the resultant graph must consist of a number of independent edges and a number of subhexagonal systems of H. Clearly, the independent edges in the resultant graph are all fixed double bonds of H. Finally, we assert that all the subhexagonal systems are normal. Otherwise, if a subhexagonal system of this kind is not normal, the sub-HS must have a fixed single bond of itself. The fixed single bond must be a fixed single bond of H because it is impossible that the fixed single bond of the sub-HS can be on an M-alternating cycle of H. Thus by theorem 3 there exist a cut or g-cut or z-cut segment of H with property (*) passing through the subhexagonal system, and therefore there must exist some red edges in the subhexagonal system, a contradiction to

the fact that the sub-HS consists of black edges. Our proof is now complete.

The following theorem gives the complexity of our algorithm.

Theorem 6: Let H be a HS, n be the number of vertices of H. Then the complexity of our algorithm is $O(n^3)$.

Proof: Let the number of hexagons of H be h. By simply counting, we know that the number of cut and g-cut and z-cut segments taken in our algorithm is at most $3h+6h+2(\frac{h(h-1)}{2})= O(h^2)$. Since $h \leq \frac{1}{4}(nn_i-2)= O(n)$ (see ref. [3]), where n_i is the number of vertices which are not on the contour of H, this implies that the number of cut and g-cut and z-cut segments taken in our algorithm is $O(n^2)$. On the other hand, for each cut or g-cut or z-cut segment, we need to count the number of peaks and the number of valleys in one of the two components of the graph obtained from H by deleting all the edges intersected by the taken cut. Obviously, to do this task takes at most n times. Therefore, the total complexity of our algorithm is $O(n^3)$.

Remark: In ref.[4] we pointed out that the number of Kekulé structures, the Clar formula and the Z-transformation graph[5] of a HS can be obtained from those of normal subhexagonal systems in H. By our algorithm, we can find all the normal subhexagonal systems in H. Thus, our algorithm can simplify the procedure of finding the number of Kekulé structures, the Clar formula and the Z-transformation graph for a HS.

IV. Concluding Remarks.

Hexagonal systems with fixed double and/or single bonds have been termed "essentially disconnected" [1,6]. Their properties are of great interest in mathematical chemistry, as is documented by a number of recent publications [7-12].

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