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CLAR FORMULA OF A CLASS OF HEXAGONAL SYSTEMS

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ABSTRACT. A hexagonal system is said to be a CHS if it can be dissected by parallel horizontal lines L_i $(i=1,2,\dots,t)$ such that it decomposes into t+1 paths. The one top and the one bottom must be of even length. All other paths must be of odd length. In this paper we discuss some topological properties of CHS and obtain a fast algorithm for finding its Clar formula C and the cardinality c of C. By the algorithm, we can easily give C and c for Ribbon, Chevron[2] etc.

A hexagonal system, denoted by HS, is a finite 2-connected plane graph whose every interior region is bounded by a regular hexagon of side length 1.

A perfect matching of a graph G is a set of disjoint edges of G covering all vertices of G. Note that perfect matching of a HS is a graph-theoretical notion which is known as "Kekulé pattern", and a HS with at least one Kekulé pattern can be regarded as the skeleton of a benzenoid hydrocarbon molecule.

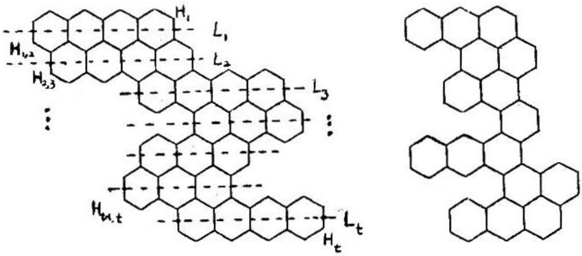
In order to simplify the discussion, we always place a HS, H, on a plane such that two edges of its each hexagon are parallel to the vertical line.

Let H be a HS, $K=\{s_1,\dots,s_m\}$ be a collection of pairwisely disjoint hexagons of H. Denote by H-K the subgraph obtained by deleting from H all the vertices of all hexagons of K together with their incident edges. We call K a cover of H, or K covers H, if either H-K has a perfect matching or it is an empty graph. A cover K of H is said to be maximum if $|K| \geq |K'|$ for any cover K' of H, and a maximum cover of H is called a Clar formula, denoted by C. The cardinality of a Clar formula of H is denoted by c(H) .

Clar formula occurs in chemistry within the so called Clar aromatic sextet theory[4]. Generally, there is no satisfactory method to find it. Now we give a fast algrithm for the Clar formula C and the cardinality c of C to a class of HS, which is described as follows.

Definition 1: Let H be a HS. H is said to be a CHS if it can be dissected by parallel horizontal lines L_i (i= 1,2,...,t) such that it decomposes into t+1 paths[5]. (as shown in Fig. 1). The one top, denoted by H_1, and the one bottom, denoted by H_t, must be of even length (the number of edges). All other paths, denoted by $H_{i,i+1}$ $(i=1,2,\ldots,t-1)$, must be of odd length. CHS is synonymous with "constructable benzenoid" described in Chapter 15 of [2].

Many classes of HS are CHS, for example, Single chains, Multiple chains, Ribbon, Chevron [2] etc. The followings are two examples of CHS.



(Fig.1)

From definition 1, the following fact is obvious. In ith row $(i=2,3,\ldots,t-1)$ of a CHS, there is one and only one of the leftest and rightest vertical edges whose top vertex is of degree 2.

For undefined terms or notions, we follow the terminology of Cyvin and Gutman [2].

SOME PROPERTIES OF CHS

Definition 2: Let H be a CHS with t rows. Draw double bonds for some vertical edges $e_1, e_2, \ldots, e_t$ of H. We say this partial matching to be exact if

(i). there is exactly one double bond e_i in the ith row of H $(i=1,2,\ldots,t)$, and

(ii). when the vertical edge with top vertex of degree 2 in the ith row is a left boundary edge, e_i must be on the left side of e_{i-1}. Otherwise, e_i must be on the right side of e_{i-1}.

Theorem 1. Let H be a CHS with t rows, $e_i(i=1,2,\ldots,t)$ be an exact partial matching of H. Then there is a unique perfect matching M of H such that $e_i(i=1,2,\ldots,t)$ are exactly its all double bonds.

Proof: Consider the subgraph H' obtained from H by deleting all vertices of $e_i(i=1,2,\ldots,t)$ together with all their incident edges. Since $e_i(i=1,2,\ldots,t)$ is an exact partial matching of H, by definition 2 we know that each of $H' \cap H_1$, $H' \cap H_t$ and $H' \cap H_{i,i+1}$ $(i=1,2,\ldots,t-1)$ must be a path with odd length or several paths with odd length. Therefore, each of them has a unique perfect matching. As a result of this fact, our conclusion is true.

Corollary 1: Let H be a CHS with t rows, then H has a perfect matching.

Proof: Chose edges $e_i(i=1,2,\ldots,t)$ as follows. e_1 is a vertical edge in the first row of H, and its two vertices are both of degree 2. e_i (i=1,2,...,t) is a vertical edge in the ith row of H, and its top vertex is of degree 2. Then e_i (i=1,2,...,t) is an exact partial matching of H and therefore H has a perfect matching.

Corollary 2: Let H be a CHS, then its $c(H) \leq$ the number of its rows.

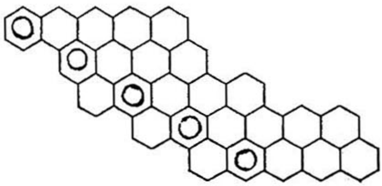
Proof: From Corollary 1 and the fact that all Kekule' structure of H have an equal number of vertical double bounds.[1] this result follows.

Theorem 2: Let H be a CHS with t rows. For any perfect matching M, its all vertical double bonds e_i (i=1,2,...,m) must be an exact partial matching of H.

Proof: From Corollary 1 and Theorem 11(Sachs) in [2], we know that m=t and there is one and only one e_i in the ith row for each i=1,2,...,t, and therefore e_i (i=1,2,...,t) satisfy condition (i) of definition 2. Now we claim that they also satisfy condition (ii) of definition 2. In fact, let $e_1,\ldots,e_{i-1}$ satisfy the condition (ii). Then if the vertical edge with top vertex of degree 2 in the ith row is a left boundary edge of H, then the vertices on the right side of e_{i-1} in $H_{i-1,i}$ are all unambiguously matched. Hence e_i can only be on the left side of e_{i-1}. Otherwise, similar reason shows that e_i can only be on the right side of e_{i-1}.

AN ALGORITHM FOR CLAR FORMULA OF SPECIAL CHS

In this section, we confine ourself to deal with such CHS whose each vertical edge with top vertex of degree 2 in all rows but the first one is a right boundary edge. We call this kind of CHS to be of A-type. An example of A-type CHS is shown in Fig.2.



(Fig.2) c = 5

ALGORITHM I: Constructing C and computimg c for A-type CHS H_1 with t rows.

Step 0: $i := 0$, $C := \emptyset$, $c(H_1) := 0$.

Step 1: $i := i+1$. If $H_i = \emptyset$, then print C and $c(H_1)$. Stop. Otherwise,

Step 2: At first, draw a proper sextet in the top-left hexagon s_i of H_i. Then, obtain a HS H_{i+1} from H_i by deleting all unambiguously matched vertices together with all their incident edges. Clearly, H_{i+1} is still a CHS. $C := C \cup \{s_i\}$, $c(H_1) := c(H_1)+1$. Go to Step 1.

Theorem 3: At the end of ALGRITHM I, C is a Clar formula of H_1 and $c(H_1)$ is is the cardinality of C.

Proof: By induction on the number t of rows of H_1. If t=1, then $H_2 = \emptyset$ and $C = \{s_1\}$, $c(H_1) = 1$. By Corollary 2, we know that our conclusion is true.

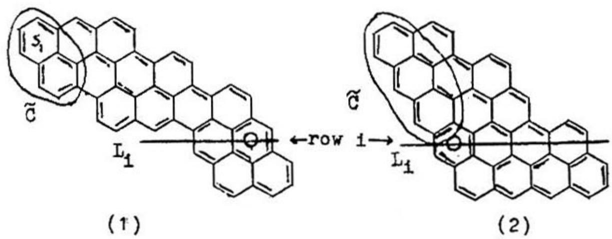
Suppose that it is true for all t such that $t < n$. Now we deal with the case of t=n.

By Theorem 1, it is easy to see that there is a unique perfect matching M of H_1 such that its all proper sextets are those hexagons of C. Hence C is a cover of H_1. Let K' be any cover of H_1 and M' be a perfect matching whose all proper sextets are exactly those hexagons of K'. We are going to prove $|C| \geq |K'|$. There are only three cases.

Case 1: The top-left hexagon s_1 of H_1 is a proper sextet of M'. Then M and M' have the same matching in $H_1 - H_2$, and s_1 is the only common proper sextet of M and M' in $H_1 - H_2$. Therefore there are $|C| - 1$ proper sextets of M and $|K'| - 1$ proper sextets of M' in H_2. Obviously, $C - \{s_1\}$ is a cover of H_2 obtained by ALGORITHM I and $K' - \{s_1\}$ is another cover of H_2. Since the number of rows of H_2 is less than n, by induction hypothesis we have $|C - \{s_1\}| \geq |K' - \{s_1\}|$, i.e., $|C| \geq |K'|$.

Case 2: There is a proper sextet of M' in the first row of H_1 but not the top-left one. Then we can move the proper sextet by transforming it into an improper one until the top-left hexagon of H_1 becomes a proper sextet. Denote the resultant perfect matching by M^*. It is not difficalt to see that the above transformations do not reduce the number of proper sextets of M'. Thus we have that the number of proper sextets of M^* is not less than $|K'|$. By Case 1, we know that the number of proper sextets of M^* is not greater than $|C|$. Hence $|C| \geq |K'|$.

Case 3: There is no proper sextet of M' in the first row of H_1. If $K' = \emptyset$, then there is nothing to say. Otherwise, from the second row on we look for proper sextet of M' row by row. Suppose the first one we encounter is in the ith row of H_1. Then the vertical double bonds in the rows before the ith row must be some left boundary edges. (as shown in Fig.3).



(Fig.3)

It is not difficalt to see that there must be an M'-alternating cycle in the upper bank of L_i. Denote such a minimal cycle containing the top-left hexagon s_1 of H_1 by $\tilde{C}$ as shown in Fig.3. Let $M^* = M' \Delta \tilde{C}$, then M^* is a perfect matching with proper sextet in the top-left hexagon s_1 of H_1. Let K^* be the set of all proper sextets of M^*. By Case 1, we have $|C| \geqslant |K^*|$. To end the proof, we need only to show that $|K^*| \geqslant |K'|$, i.e, the transformation from M' to M* does not reduce the number of proper sextets of M'. There are only two subcases.

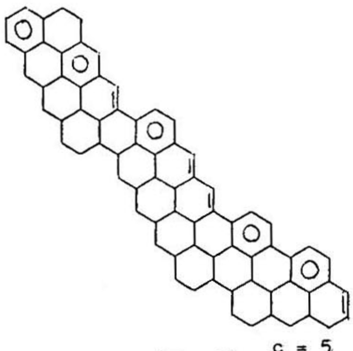
Subcase 2.1: $\tilde{C}$ has no common edge with the proper sextet in the ith row. Then the transformation from M' to M* does not affect the proper sextet in the ith row and the lower bank of L_i. Meanwhile, we obtain a new proper sextet s_1. Hence $|K^*| > |K'|$. (shown in Fig.3 (1)).

Subcase 2.2: $\tilde{C}$ has an edge in common with the proper sextet in the ith row. (shown in Fig.3 (2)). Then the transformation from M' to M* reduce the proper sextet in ith row to an improper one. On the other hand, we obtain a new proper sextet in the top-left hexagon s_1. Hence we have $|K^*| = |K'|$.

Our proof is now completed.

Remark 1: If we change the word "right" into " left" in the definition of A-type CHS, then similar algorithm is effective.

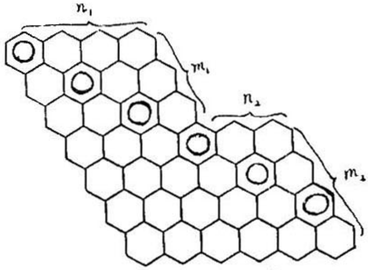
Remark 2: When using ALGORITHM I , we need not to know any subgraphs $H_2, H_3, \ldots,$ and we can draw a series of circles on a given A-type CHS as far left as possible until such circles can not be drawn. Then, we draw a series of vertical double bonds until we can draw circles again. Repeat the above procedure until the bottom row of H_1 is reached. At last, the all drawn circles from a Clar formula of CHS H_1. An example is as shown in Fig.4.



(Fig.4)

Corollary 3: Let $R(n_1, n_2; m_1, m_2)$ be a Ribbon[2] shown in Fig.5. Then its $c(R(n_1,n_2;m_1,m_2))=$

$$\begin{cases} n_1+\min\{n_2,m_2\}, & \text{for } n_1<m_1. \\ \min\{n_1+n_2,m_1+m_2\}, & \text{otherwise.} \end{cases}$$

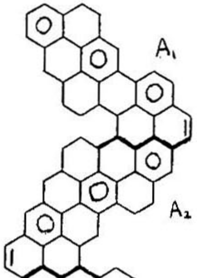


c = 6

(Fig.5)

AN ALGORITHM FOR CLAR FORMULA OF GENERAL CHS

It is obvious that a general CHS can be decomposed into some pieces of A-type CHS $A_1,A_2,\ldots,A_m$ shown as in Fig.6.



(Fig.6) c = 8

Note that there exists a vertical edge with both vertices of degree 2 in the first row of any CHS H.

ALGORITHM II

Input: Let H_1 be a CHS. It is built up as shown in Fig.6.

Output: A Clar formula C and $c(H_1)$ of H_1.

Step 0: $i := 0$, $C := \emptyset$, $c(H_1) := 0$.

Step 1: $i := i+1$. If $H_i = \emptyset$, then print C and $c(H_1)$. Stop. Otherwise,

Step 2: At first, in the first row of H_i draw a proper sextet s_i in the hexagon having an edge with both vertices of degree 2. Then obtain a subgraph H_{i+1} from H_i by deleting all unambiguously matched vertices together with all edges incident to them. Obviously, H_{i+1} is still a CHS. $C := C \cup \{s_i\}$, $c(H_1) := c(H_1) + 1$. Go to Step 1.

Theorem 4: At the end of Algorithm II, C is a Clar formula of H_1 and $c(H_1)$ is the cardinality of C.

Proof: The arguments similar to the proof given in Theorem 3 are valid. We do not repeat them here.

Remark 3: Both ALGORITHM I and II can end in a finite number of circulations. Actually, the number of circulations is not greater than the number of rows of H_1. Therefore, they are good algorithms.

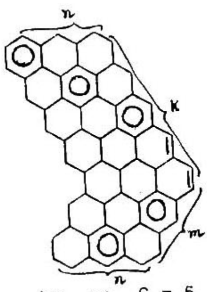
Remark 4: When using ALGORITHM II, we also need not to know any Subgraphs $H_2, H_3, \ldots,$ and we can draw circles directly on a given CHS H_1, similar to Remark 1. (see Fig.6).

Corollary 4: Let H be a CHS and built up with A-type CHS $A_1, A_2, \ldots, A_m$. Then we have the following inequality:

$$\sum_{i=1}^{m} c(A_i) - m + 1 \leq c(H) \leq \sum_{i=1}^{m} c(A_i) .$$

Corollary 5: Let CH(k,m,n) be a Chevron [2] as shown in Fig.7. Then its $c(CH(k,m,n)) =$

$$\begin{cases} \min\{n,k\} + \min\{n,m\}, & \text{for } n > k \text{ or } n > m, \\ 2n-1, & \text{otherwise.} \end{cases}$$



(Fig.7) c = 5

CONCLUSION

Let $H_1, H_2, \ldots, H_m$ be m CHS. We obtain a HS H from them by joining some valleys on the bottom of H_i with some peaks on the top of H_{i+1}. Then H is no longer a CHS. Since the vertical edges of H between H_i and H_{i+1} must be fixed single bonds, we can deal with H_i one by one firstly, and then we have that

$$C(H)= C(H_1)\cup C(H_2)\cup \ldots \cup C(H_m),$$

and $$c(H)= c(H_1)+ c(H_2)+ \ldots + c(H_m).$$

where $C(H_i)$ denotes a Clar formula of H_i, and $c(H_i)$ is the cardinality of $C(H_i)$.

Prolate Rectangle[2] is an example of this kind of structure.

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