match no. 19 pp. 179-188 1986

A THEOREM CONCERNING POLYHEX GRAPHS

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(Received: Spetember 1985)

Abstract

We establish a theorem which offers a characterization of polyhex graphs with the property that the number of Kekulé patterns is equal to the number of generalized Clar formulas plus one.This is a generalization of a previous result by Gutman,Hosoya,Yamaguchi,Motoyama and Kuboi.

In the present paper we consider polyhex graphs. A polyhex graph,also called "benzenoid system" or "hexagonal system",corresponds to a network obtained by arranging congruent regular hexagons in the plane so that two hexagons are either disjunct or possess a common edge.For a more precise definition of polyhex graphs, the reader is refered to [1]. Throughout this paper we confine ourselves to those polyhex graphs which have at least one Kekulé pattern (KP). Note that a KP is just a chemical notion which coincides with what is known in graph theory under the name "1-factor".

Let G be a polyhex graph, H be a subgraph of G. We use G-H to denote the subgraph of G obtained by deleting from G all the vertices of H together with their incident edges. Let $K=\{s_1, \ldots, s_t\}$ $(t \geq 1)$ be a collection of disjunct hexagons of a polyhex graph G. If G-K has a 1-factor, then K is said to be a generalized Clar formula (GCF). In the case when G-K is an empty graph, we assume that G-K has a 1-factor. A GCF is a concept which occurs in chemistry, within the so called Clar aromatic sextet theory. For more details along these lines see refs. [1,2].

A polyhex graph G is called a catahex if no three hexagons of G have a point in common. A polyhex graph not being a catahex is called a perihex.

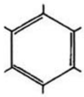
Hosoya and Yamaguchi [5] observed an interesting property of catahexes, which in the terminology of the present paper can be stated as follows. If G is a catahex and has f KPs, then G has f-1 GCFs.

The above result has been proved by Gutman et al. [4]. But counterexamples show that this result cannot be simply extended to perihexes. As an attempt, Gutman [3] formulated a conjecture that if a perihex G has a Hamiltonian cycle and has f KPs, then G has f-1 GCFs. Unfortunately, this conjecture is invalid [8]. The authors of [7] have extended the above result to a class of perihexes.It is natural to ask when a perihex graph G has the following property.

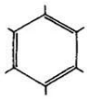
Property (*) The number of GCFs is equal to the number of KPs minus one.

The main aim of this paper is to characterize those perihexes which have Property (*).

For brevity,a perihex in question is to be placed on a plane so that two edges of each hexagon are parallel to the vertical line.The sets of three circularly arranged double bonds in a given KP are called proper and improper sextets, respectively [6].(see Fig.1)



proper sextet



improper sextet

Fig.1

Let A be the set of all KPs of a perihex G,B be the set of all GCFs of G.It is not difficult to see that for any KP M in A,there is an associate set K (possibly,$K=\emptyset$) consisting of proper sextets of M.If $K\neq\emptyset$,then K is evidently a GCF of G. Therefore $K \in B\cup\{\emptyset\}$.We now set up a mapping g from A to $B\cup\{\emptyset\}$. For any $M \in A$,we define the image of M under the mapping g as K,and write $g(M)=K$.

In order to establish our main theorem,we need the following lemmas.

Lemma 1. [7] For each $K\in B\cup\{\emptyset\}$,there is at least one $M \in A$ such that $g(M)=K$.

Lemma 2. Let G be a perihex with exterior boundary P, M_1 and M_2 be two 1-factors of P. If $G-P$ has a 1-factor M and $g(M\cup M_1)=g(M\cup M_2)$, then G has a coronene C as its subgraph such that $G-C$ has a 1-factor.

Proof. By contradiction. Suppose that the lemma is false. Then there exist perihexes $\{G_i, i=1,\ldots\}$ satisfying the conditions in the lemma and possessing no coronene subgraph C_i, such that G_i-C_i has a 1-factor. Among those perihexes we can pick out one (denoted by G) with minimal number of hexagons, i.e., any proper subgraph G' of G will not be in $\{G_i, i=1,\ldots\}$.

We can take a series of hexagons $\{s(i,j) \mid 1 \leq i \leq m, 1 \leq j \leq n(i)\}$, as shown in Fig.2, which lie on the boundary of the exterior region of G, and satisfy the condition that neither the hexagon L nor the hexagon N is contained in G. We denote the hexagon next to $s(i,n(i))$, if any, by $T(i-1)$, $i=2,\ldots,m$ (see Fig.2).

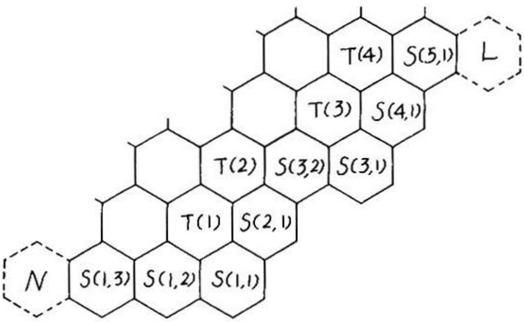


Fig.2 Hexagons $s(i,j)$ and $T(i)$ with $n(1)=3$, $n(2)=1$, $n(3)=2$, $n(4)=n(5)=1$ and $m=5$. $N, L \notin G$.

We first show that $n(1) \leqslant 2$ and $T(1) \in K$ when $n(1)=2$. Without loss of generality, we may assume that the edge e (see Fig.3) is contained in M_1. Now if $n(1) \geqslant 3$, then $e^* \notin M$. Otherwise, $s(1,1) \in g(M \cup M_1)$ and $s(1,1) \notin g(M \cup M_2)$, contradicting $g(M \cup M_1) = g(M \cup M_2)$. Thus in the case when $T(1) \notin K$, we have $e(1,2), \ldots, e(1,n(1)) \in M$. While in the case $T(1) \in K$, we have $e(1,3), \ldots, e(1,n(1)) \in M$. We now denote by G^* the subgraph of G obtained by deleting from G the edge e together with its two endpoints. Let P^* be the exterior boundary of G^*. One can check that $M^* = M - e(1,n(1))$ is a 1-factor of $G^* - P^*$. Thus $M_1^* = (M_1 - \{e\}) \cup \{e(1,n(1))\}$ and $M_2^* = (M_2 - \{e_1, e_2\}) \cup \{e_3, e_4\}$ are two 1-factors of P^* (see Fig.3). Since e_3 and e_4 cannot be edges of proper sextets, we have $g(M^* \cup M_1^*) = g(M^* \cup M_2^*) = K$. G^* has no coronene C^* as its subgraph such that $G^* - C^*$ has a 1-factor since G^* is a subgraph of G. Therefore G^* is a member of $\{G_i, i=1,\ldots\}$, contradicting the minimality of G. Consequently, $n(1) \leqslant 2$. By an analogous argument, we have $T(1) \in K$ when $n(1)=2$.

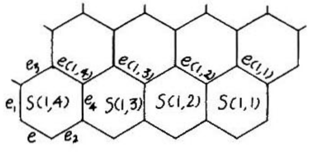


Fig.3 Edges $e(1,j)$ with $j=1,\ldots,n(1)$, where $n(1)=4$.

We now distinguish two cases.

Case 1. $n(1)=2$ and $T(1) \in K$. There is no loss in generality in assuming that the edges a, b, c and d are contained in M_1 (see

Fig.4).If $n(2)\geqslant 2$,then there is a series of edges of $M\cup M_1$ $r(1,1),r(1,2),\ldots,r(1,h(1));r(2,1),r(2,2),\ldots,r(2,h(2));\ldots\ldots;$ $r(s,1),r(s,2),\ldots,r(s,h(s))$,as shown in Fig.4.We can find one or two $M\cup M_1$ alternating cycles in G (i.e.,cycles whose edges are alternately in $M\cup M_1$ and $E(G)-M\cup M_1$,where $E(G)$ is the edge set of G),namely $Q_i, i\in I, I=\{1\}$ or $\{1,2\}$(see Fig.4).Let $M'=(M\cup M_1)\cup(\bigcup_{i\in I}Q_i)-(M\cup M_1)\cap(\bigcup_{i\in I}Q_i)$.One can check that M' is another 1-factor of G.Then we can get a coronene C as a subgraph of G such that G-C has a 1-factor $(G-C)\cap M'$,as shown in Fig.4.This contradicts the hypothesis.Now if $n(2)=1$,we can discuss similarly and also obtain a desired contradiction.

Case 2. $n(1)=1$. If $n(i)=1$ for $1\leqslant i\leqslant m-1$,then $e_2\in M$(see Fig.5). (If $e_2\in M_1$,then $s(1,1)\notin g(M\cup M_1)$ and $s(1,1)\in g(M\cup M_2)$,a contradiction.)Hence $e_3,\ldots,e_{m-1}\in M$.Thus there is a proper subgraph G' of G as shown in Fig.5.It is not difficult to check that G' is in $\{G_i, i=1,\ldots\}$,contradicting the minimality of G. Consequently,there exists a number j such that $2\leqslant j\leqslant m-1$ and $n(j)\geqslant 2$.If $n(j)\geqslant 3$ or $n(j)=2$ but $T(j-1)\notin K$,then edge $e'\in M$ (see Fig.6).Let $G^*=G-\{e\}$.One can check that G^* is in $\{G_i, i=1,\ldots\}$,a contradiction.Therefore $n(j)=2$ and $T(j-1)\in K$.Now by a similar argument as in the case 1,we get a coronene C as a subgraph of G such that G-C has a 1-factor,still a contradiction.

Each case leads to a desired contradiction.Consequently, the lemma is proved.

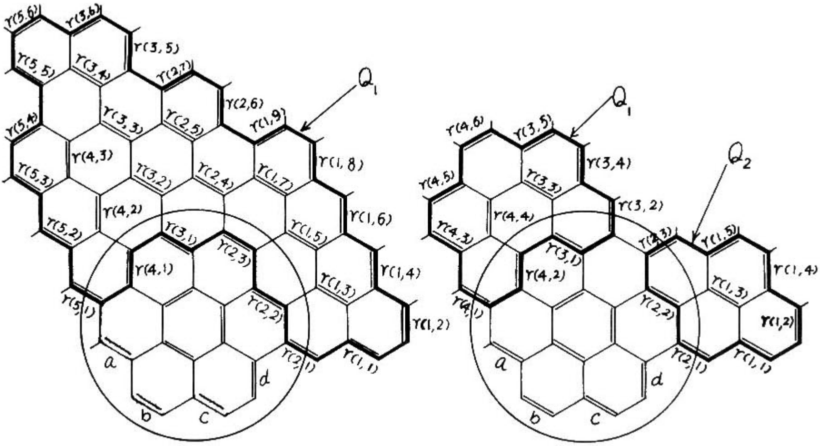


Fig.4 Edges r(i,j) and MUM$_1$ alternating cycle Q_i.

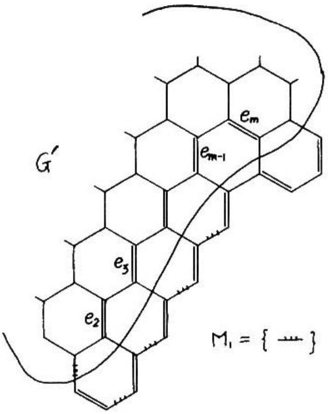


Fig.5 Subgraph G' of G.

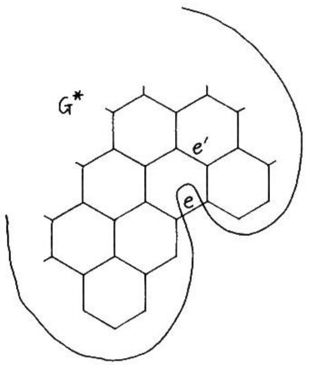


Fig.6 Subgraph G* of G.

We are now in the position to prove our main result.

<u>Theorem</u>. A perihex G possesses Property (*) if and only if for any coronene C which is a subgraph of G, G-C has no 1-factor.

<u>Proof.</u> Suppose that G has a coronene C as its subgraph and G-C has a 1-factor M. Let M_1 be a 1-factor of C as shown in Fig.7. Evidently, $M \cup M_1$ is a 1-factor of G. Starting with the center of the hexagon s, we divide the plane into three areas 1,2 and 3 (see Fig.7). It is not difficult to see that there exists a subgraph H of G satisfying the following conditions.

(1) C is a subgraph of H (or H=C).

(2) If $M^* = H \cap (M \cup M_1)$, then M^* is a 1-factor of H.

(3) If edge $e \in M$ and e is contained in the area i, then e is parallel to e_i for i=1,2 and 3.

(4) The perimeter P of H is an alternating cycle with respect to the edges of M.

(5) H is maximal, i.e., there is no subgraph of G satisfying the above four conditions and containing H as a proper subgraph.

Now let $K = g(M \cup M_1)$. Evidently, $s \in K$, where s is the hexagon indicated on Fig.7. Let $M' = (M \cup M_1) \cup P - (M \cup M_1) \cap P$. Then M' is another 1-factor of G and we can easily check that $g(M') = g(M \cup M_1) = K$. This together with the fact described in Lemma 1 yields $|A| > |B| + 1$. (For a set X, $|X|$ denotes the cardinality of X)

Conversely, if $|A| > |B| + 1$, then there are two 1-factors M_1 and M_2 of G such that $g(M_1) = g(M_2)$. As a well-known fact, the symmetric difference $M_1 \triangle M_2 = M_1 \cup M_2 - M_1 \cap M_2$ is the union of some disjoint (M_1, M_2) alternating cycles (i.e., the cycles whose edges

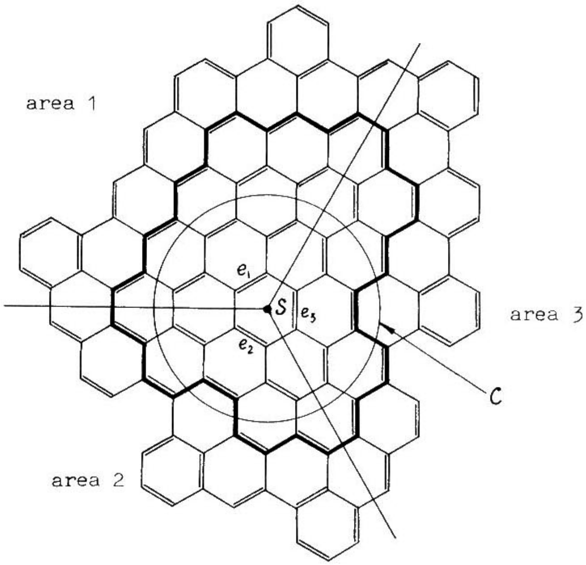


Fig.7 Subgraph H of G.(H is surrounded by bold lines.)

are alternately in M_1 and M_2).Let P be one of them such that there is no (M_1,M_2) alternating cycle inside it.Let then G' be the subgraph of G whose exterior boundary is P.It is not difficult to see that $M'=M_1\cap(G'-P)=M_2\cap(G'-P)$ is a 1-factor of G'-P,whereas $M_1'=M'\cup(M_1\cap P)$ and $M_2'=M'\cup(M_2\cap P)$ are two 1-factors of G'.Furthermore,$g(M_1')=g(M_2')=K\cap G'$.Thus by Lemma 2,there is a coronene C as a subgraph of G' such that G'-C has a 1-factor M". Consequently,C is a subgraph of G and G-C has a 1-factor $M''\cup(M_1\cap E(G-G'))$.The proof is complete.

<u>Corollary</u>. 7 If G is a thin perihex,then G has Property (*).

REFERENCES

(1) I.Gutman,Topological properties of benzenoid systems,Bull. Soc. Chim. Beograd 47(1982),453-471.

(2) I.Gutman,Topological properties of benzenoid systems,XIX. Contributions to the aromatic sextet theory,Wiss. Z. TH Ilmenau 29(3) (1983),57-65.

(3) I.Gutman,Covering hexagonal systems with hexagons,in: Proceedings of the Fourth Yugoslav Seminar on Graph Theory, Novi Sad ,1983.

(4) I.Gutman,Hosoya,T.Yamaguchi,A.Motoyama and N.Kuboi, Topological properties of benzenoid systems,III. Recursion relation for the sextet polynomial,Bull. Soc. Chim. Beograd 42 (1977),503-510.

(5) H.Hosoya and T.Yamaguchi,Sextet polynomial,Tetrahedron Letters (1975),4659-5662.

(6) N.Ohkami,A.Motoyama,T.Yamaguchi,H.Hosoya and I.Gutman, Graph-theoretical analysis of the Clar's aromatic sextet, Tetrahedron 37 (1981),1113-1122.

(7) F.J.Zhang,R.S.Chen and M.L.Zheng,Graph-theoretical results of the Clar's aromatic sextet,to be submitted to Graphs and Combinatorics.

(8) R.S.Chen et al.,Counterexamples to Gutman's conjecture concerning hexagonal systems,J.Xinjiang University 1 (1985), 12-14.