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Essentially Disconnected Character of Essentially Disconnected Coronoid Systems [1]

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Abstract

An essentially disconnected coronoid system is defined as a Kekuléan coronoid system which has fixed (single or double) bonds and has at least one hole. It is proved that the subgraph, obtained by deleting all the fixed single bonds and all the end vertices of the fixed double bonds, is disconnected, and has at least two normal components, which generalizes the result for essentially disconnected benzenoid systems by Gutman et al [4].

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1. Introduction

A benzenoid system [1] is a finite connected subgraph of the infinite hexagonal lattice without cut vertices or non-hexagonal interior faces. A coronoid system [2] is a subgraph of a benzenoid system and has at least one "hole", i.e. a non-hexagonal interior face. Coronoid systems are divided into single coronoid systems (i.e. coronoid systems with exactly one hole) and multiple coronoid systems (i.e. coronoid systems with more than one hole). Benzenoid systems and coronoid systems are widely used because they are the representations of the skeletons of molecules of benzenoid hydrocarbons and coronoid hydrocarbons. A benzenoid system H and a single coronoid system G obtained from H are depicted in Fig.1 , and a multiple coronoid system is depicted in Fig.2.

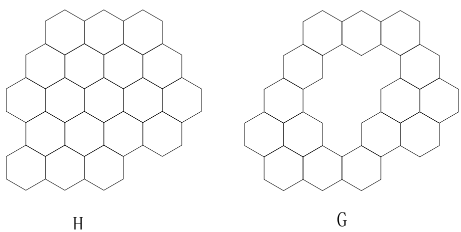

Fig.1 A benzenoid system H and a coronoid system G obtained from H

A polyhex graph is either a benzenoid system or a coronoid system. A Kekulé structure of a polyhex graph G is a set of disjoint edges of G which cover all the vertices of G. A Kekuléan polyhex graph is a polyhex graph with Kekulé structures. For a Kekuléan polyhex graph G and a Kekulé structure M of G, an M-alternating cycle is a cycle whose edges are alternately in M and $E(G) - M$, where $E(G)$ is the edge set of G. An edge of a Kekuléan polyhex graph G is a fixed single (double) bond if it belongs to none (all) of the Kekulé structures of G. A fixed bond is either a fixed single bond or a fixed double bond. A polyhex graph with fixed bonds is said to be an essentially disconnected polyhex graph [3]. Otherwise, it is said to be a normal polyhex graph.

The structural feature of essentially disconnected benzenoid system is already known [4-6]. For an essentially disconnected benzenoid system, after deleting all the fixed double bonds together with their end vertices and all the fixed single bonds without their end

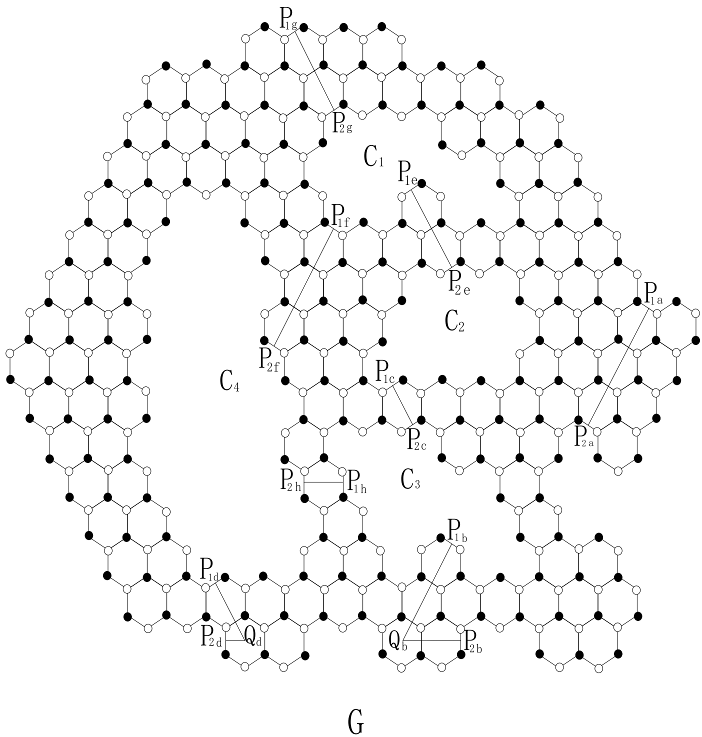

Fig.2 A multiple coronoid system G with four holes

vertices, there are at least two components which are normal benzenoid systems. The aim of the present paper is to generalize the result to essentially disconnected coronoid systems.

2. Definitions and notations

Let G be a coronoid system, C_0 the outer perimeter of G (i.e. the perimeter of the corresponding benzenoid system), $C_1, C_2, \cdots, C_k$ the inner perimeters of G (i.e. the perimeters of the holes). Since the concept of special edge cut plays an important role in our investigation, we give the following definitions.

Definition 1 [6] A straight line segment P_1P_2 is called an elementary cut segment($e-$cut segment) from C_i to C_j if:

1. P_1 is the center of an edge e_i on C_i, and P_2 is the center of an edge e_j on C_j;
2. P_1P_2 is orthogonal to both e_i and e_j;
3. any point of P_1P_2 is either an interior or a boundary point of some hexagon of G.

The set of all the edges intersected by an elementary cut segment P_1P_2 is called an elementary cut corresponding to P_1P_2.

Definition 2 [6] A broken line segment P_1QP_2 is called a generalized cut segment($g-$cut segment) from C_i to C_j if:

1. P_1 is the center of an edge e_i on C_i, P_2 is the center of an edge e_j on C_j, and Q is the center of some hexagon of G;
2. P_1Q and P_2Q are orthogonal to e_i and e_j respectively and the angle P_1QP_2 is $60°$ or $300°$;
3. any point of P_1QP_2 is either an interior or a boundary point of some hexagon of G.

The set of all the edges intersected by a $g-$cut segment P_1QP_2 is called a $g-$cut corresponding to P_1QP_2.

Definition 3 A special edge cut is either an $e-$cut or a $g-$cut from C_i to C_j, denoted by E_{ij}.

It is obvious that each special edge cut E_{ij} has exactly two edges on the perimeters of G. E_{ij} is said to be of type I if $i = j$. Otherwise E_{ij} is said to be of type II.

Since a polyhex graph G is bipartite, in the following, we may assume that the vertices of G is colored black and white such that any two adjacent vertices of G are differently colored. We denote the sets of white and black vertices of G by $W(G)$ and $B(G)$, respectively.

Definition 4 [6] Let $E_{i_1i_2}$, $E_{i_2i_3}$, $\cdots$, $E_{i_{t-1}i_t}$, $E_{i_ti_1}$ be t pairwise disjoint special edge cut of type II corresponding to an $e-$cut or $g-$cut segment from C_{i_j} to $C_{i_{j+1}}$ and $i_1 \neq i_2 \neq \cdots \neq i_t$; $E = E_{i_1i_2} \cup E_{i_2i_3} \cup \cdots \cup E_{i_{t-1}i_t} \cup E_{i_ti_1}$. E is said to be a standard combination if the end vertices of the edges of E have the same color when they lie in the same component of $G - E$, where $G - E$ is the subgraph obtained from G by deleting all the edges of E.

In Fig.2, let E_{01} be the $g-$cut corresponding to the $g-$cut segment $P_{1d}Q_dP_{2d}$, E_{12} the $e-$cut corresponding to the $e-$cut segment $P_{1h}P_{2h}$, E_{23} the $e-$cut corresponding to the $e-$cut segment $P_{1c}P_{2c}$, E_{34} the $e-$cut corresponding to the $e-$cut segment $P_{1e}P_{2e}$, E_{40} the $e-$cut corresponding to the $e-$cut segment $P_{1g}P_{2g}$. Then $E = E_{01} \cup E_{12} \cup E_{23} \cup E_{34} \cup E_{40}$ is a standard combination. While the three $e-$cuts corresponding to $e-$cut segments $P_{1g}P_{2g}$, $P_{1e}P_{2e}$ and $P_{1c}P_{2c}$, respectively, and the g-cut corresponding to the g-cut segment $P_{1b}QP_{2b}$ do not constitute a standard combination.
In [6], a necessary and sufficient condition for a Kekuléan coronoid system to be essentially disconnected was given.

Theorem 1 [6] Let G be a Kekuléan coronoid system, C_0 the outer perimeter of G, C_1,$\cdots$,$C_k (k \geq 1)$ the inner perimeters of G. Then G is essentially disconnected if and only if G possesses a special edge cut R of type I, or a standard combination E of type II, satisfying: $|B(\mathrm{G}_1)| = |W(G_1)|$ and $|B(G_2)| = |W(G_2)|$, where $G_i (i = 1, 2)$ are the two components of $G - R$ or $G - E$.

The above theorem implies that for an essentially disconnected coronoid system G, after deleting the fixed single bonds which form a special edge cut R of type I or a standard combination E of type II, the subgraph $G - R$ or $G - E$ is disconnected and has at least two components.

3. Main results

Let G be a polyhex graph, A a set of vertices of G. $G-A$ designates the subgraph obtained by deleting all the vertices of A together with their incident edges.

Lemma 1 Let G be a coronoid system, C_0 the outer perimeter of G, $C_1, \cdots, C_k$ the inner perimeters of G. Let $v_1, \cdots, v_s$ be s vertices simultaneously on some perimeter C_t of G, $A = \{v_1, \cdots, v_s\}$. Suppose that in $G-A$, the perimeter C_t is broken into s segments with even lengths. If $G-A$ has a Kekulé structure M, then $G-A$ has an M-alternating cycle.

Proof: Assume that G has n vertices, m edges, k holes and h hexagons. We may further assume that G has p external edges (i.e. the edges lying on the perimeters of G), then G has $m-p$ internal edges (i.e. the edges not lying on the perimeters of G). Evidently, each internal edge belongs to two hexagons. Thus we have:

$$6h = 2(m-p) + p, \qquad \text{i.e.}$$

$$m = 3h + p/2. \tag{1}$$

By Euler formula which says that for a connected plane graph, the number of vertices plus the number of faces is equal to the number of edges plus two[7], we have:

$$n + (h + k + 1) = m + 2, \qquad \text{i.e.}$$

$$n - m + h = 1 - k, \tag{2}$$

which together with (1) yields the following:

$$n - 2h - p/2 = 1 - k, \tag{3}$$

Suppose that M is a Kekulé structure of $G-A$. If there are r external edges of G in M, then there are $(n-s)/2 \; - r$ internal edges of G in M. By the assumption, in $G-A$

the perimeter C_t of G is broken into s segments each of which contains even number edges. Let r_i be the number of edges on perimeter C_i which are contained in M, p_i the number of edges on perimeter C_i. Therefore, we have: $r = r_0 + r_1 + r_2 + \cdots + r_k$, $p = p_0 + p_1 + p_2 + \cdots + p_k$, $r_t \leq (p_t - 2s)/2$ and $r_j \leq p_j/2$ $(j \neq t, 0 \leq j \leq k)$. If some of the perimeters $C_0, C_1, \cdots, C_k$ is an M-alternating cycle, then there is nothing to prove. Now suppose that none of the perimeters $C_0, C_1, \cdots, C_k$ is an M-alternating cycle. Thus, we have $r_t \leq (p_t - 2s)/2$ and $r_j \leq p_j/2 \quad - 1 \quad (j \neq t, 0 \leq j \leq k)$. Therefore,

$$r = r_0 + r_1 + r_2 + \cdots + r_k \leq \frac{P_t - 2s}{2} + \sum_{j \neq t}(\frac{P_j}{2} - 1) = \sum_{j=0}^{k}(\frac{P_j}{2}) \quad - s - k = p/2 \quad - \quad s - k,$$

i.e.

$$r \leq p/2 - s - k, \tag{4}$$

If none of the hexagons of $G - A$ is an M-alternating cycle, then at most two edges of each hexagon of G belong to M. Hence we have: $2h \geq r + 2((n - s)/2 - r)$,
i.e.

$$2h \geq n - r - s, \tag{5}$$

Bearing in mind the inequality (4), we have: $2h \geq n - r - s \geq n - p/2 + k$, i.e. $n - 2h - p/2 \leq -k$, which contradicts (3). This contradiction implies that $G - A$ has at least one hexagon being an M-alternating cycle if none of the perimeters $C_0, C_1, \cdots, C_k$ is an M-alternating cycle.

The lemma is thus proved.

Lemma 2 Let G be a benzenoid system, C_0 the perimeter of G. Let $v_1, \cdots, v_s$ be s vertices simultaneously on C_0, $A = \{v_1, \cdots, v_s\}$. Suppose that in $G - A$, the perimeter C_0 is broken into s segments with even lengths. If $G - A$ has a Kekulé structure M, then $G - A$ has an M-alternating cycle.

The proof of the above lemma is analogous to that of Lemma 1. In other words, if one puts $k = 0$ in the proof of Lemma 1, one can reach the conclusion for benzenoid systems.

In the following we introduce a special kind of graphs called generalized coronoid system. A generalized coronoid system G is a subgraph of a benzenoid system H and has at least one hole with at least one edge not belonging to any hexagon of G (see Fig.3).

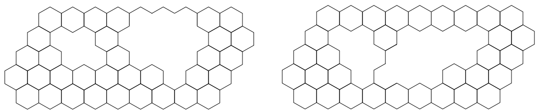

Fig.3 Two generalized coronoid systems with two holes

Lemma 3 Let G be a generalized coronoid system, C_0 the outer perimeter of G, $C_1, \cdots, C_k$ the inner perimeters of G, $v_1, \cdots, v_s$ be s vertices simultaneously on some perimeter C_t of G, $A = \{v_1, \cdots, v_s\}$. Suppose that in $G - A$, the perimeter C_t is broken into s segments with even lengths. If $G - A$ has a Kekulé structure M, then $G - A$ has an M-alternating cycle.

The proof of the above lemma is fully analogous to that of lemma 1. Hence we omit the details.

By lemmas 1-3, if we put $A = \phi$, i.e. $s = 0$ in the proof of the lemmas, we immediately have the following result.

Lemma 4 Let G be a polyhex graph or a generalized coronoid system with a Kekulé structure M, then G has an M-alternating cycle.

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

Theorem 2 If G is an essentially disconnected coronoid system, then the subgraph from G obtained by deleting all the fixed single bonds and all the end vertices of the fixed double bonds is disconnected.

Proof: By theorem 1, G has a special edge cut R of type I or a standard combination

E of type II such that the edges of R or E are fixed single bonds. Then after deleting all the fixed single bonds of R or E, G has at least two components G_1 and G_2. Each of them may be a component with or without one pendent edge; with or without one hole. In the following, we prove that each component G_i has some non-fixed bonds, i.e. G_i has a normal component which is also a normal component of G . We distinguish two cases:

Case 1. Suppose that G_i has no pendent edge. Then G_i is itself a benzenoid system, or a coronoid system , or a generalized coronoid system. Thus by lemma 4, G_i has some non-fixed bonds (note that all the edges on an M-alternating cycle are non-fixed bonds). Thus, after deleting all the fixed single bonds and all the end vertices of the fixed double bonds, G_i has a component consisting of non-fixed bonds, i.e. a normal component. Evidently, this normal component is also a normal component of G and is a normal benzenoid system or a normal coronoid system , or a normal generalized coronoid system.

Case 2. Suppose that G_i has some pendent edges, say $u_{ij}v_{ij}(j = 1, 2, \cdots, s)$, where u_{ij} is a vertex of degree 1 in G_i. Since G is a Kekuléan coronoid system and all the edges of R or E are fixed single bonds, all the pendent edges $u_{ij}v_{ij}$ $(j = 1, 2, \cdots, s)$ of G_i are fixed double bonds. By deleting all the pendent edges $u_{ij}v_{ij}$ $(j = 1, 2, \cdots, s)$ together with the end vertices u_{ij}, we obtain a benzenoid system, or a coronoid system, or a generalized coronoid system G_i^*. Put $A_i = \{v_{i1}, v_{i2}, \cdots, v_{is}\}$. Then $G_i^* - A_i$ has a Kekulé structure. Keep in mind the definitions of special edge cut of type I and the standard combination of type II, one can easily check that A_i satisfies the condition in lemmas 1-3. Therefore, $G_i^* - A_i$ has some non-fixed bonds. Consequently, $G_i^* - A_i$ has at least a normal component which is also a normal component of G and is a normal benzenoid system or a normal coronoid system , or a normal generalized coronoid system..

So we now come to the conclusion that G has at least two normal components, one from G_1, and the other from G_2. Each of them may be a normal generalized coronoid system, or a normal coronoid system, or a normal benzenoid system.

The theorem is thus proved.

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