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Essentially Disconnected Polyhexes [1]

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Abstract: A polyhex is either a benzenoid system or a coronoid system. A Kekuléan polyhex is a polyhex with Kekulé structures. An essentially disconnected polyhex is a Kekuléan polyhex with fixed bonds. Polyhexes and their Kekulé structures represent the molecules of certain aromatic hydrocarbons and their Kekulé patterns, respectively. In this paper, a uniform criterion is given to recognize essentially disconnected polyhexes.

INTRODUCTION

A benzenoid system[1] is a finite 2-connected plane graph in which every interior face is bounded by a regular hexagon of side length 1. Coronoid systems[2] can be regarded as a sort of benzenoid systems with holes. A coronoid system G can be obtained from a benzenoid system H by deleting all the vertices and edges in the interior of a group of pairwise disjoint cycles $C_1, C_2, \cdots, C_m (m \geq 1)$ which are inside H, i.e. C_i contains no vertex on the boundary of H. These cycles are called the inner boundaries of G, while the boundary C_0 of H is called the outer boundary of G, or simply, the boundary of G. If G has exactly one inner boundary, G is called a single coronoid system; otherwise, G is called a multiple coronoid system. A coronoid system is either a single coronoid system or a multiple coronoid system.

The term "polyhex" [2] is used to denote benzenoid systems and coronoid systems together. Polyhexes are of great chemical relevance[1,2] since they are the natural graph representations of the skeletons of benzenoid hydrocarbons and coronoid hydrocarbons. Research in this area has attracted the constant attention of both chemists and mathematicians.

Recall that a Kekulé structure of a polyhex G is an independent edge set of G such that every vertex of G is incident with an edge in the set. Kekulé structures play a more or less significant role in numerous chemical theories, of

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which the resonance theory and the valence bond theory are the best known examples [3]. A Kekuléan polyhex is a polyhex with Kekulé structures.

It may happen that an edge of a kekuléan polyhex in a particular position is always or never selected in all the Kekulé structures of that kekuléan polyhex. The fixed double or single bonds are just associated with such edges. The existence of fixed bonds has been known to chemists [4,5]for a long time. Cyvin and Gutman are the first to use the term "essentially disconnected" [6] to indicate those kekuléan polyhexes with fixed bonds. Later the authors of [8] strictly proved that the subgraph , obtained from an essentially disconnected polyhex by deleting all the fixed single bonds and all the end vertices of the fixed double bonds, is disconnected. This is just what the term "essentially disconnected" means.

The concept "essentially disconnected" has proved to be very useful in certain enumeration techniques for kekulé structures [7], and in classification and enumeration of kekuléan polyhexes [8]. Many attempts have been made to recognize essentially disconnected polyhexes [6-16]. Several methods have been reported to find fixed bonds in Kekuléan polyhexes. In the past, essentially disconnected benzenoid systems and essentially disconnected coronoid systems were dealt with separately. This is mainly because coronoid systems are not simply connected [1]. So, many elegant and powerful statements valid for benzenoid systems do not hold for coronoid systems.

In this paper, a uniform approach is given to recognize essentially disconnected polyhexes, whether they are benzenoid systems or coronoid systems.

DEFINITIONS

let G be a polyhex. Denote the outer boundary of G by C_0 , and by $C_1, C_2, \cdots, C_m$ the inner boundaries of G (if any).

Definition 1[11] A straight line segment P_1P_2 is called an elementary cut segment from C_i to C_j if

1. P_1 is the center of an edge e_1 on C_i and P_2 is the center of an edge e_2 on C_j;
2. P_1P_2 is orthogonal to both e_1 and e_2;
3. any point of P_1P_2 is either an interior or a boundary point of some hexagon of G.

Definition 2 [11] A broken line segment P_1QP_2 is called a generalized cut segment from C_i to C_j if

1. P_1 is the center of an edge e_1 on C_i and P_2 is the center of an edge e_2 on C_j;
2. P_1Q and P_2Q are orthogonal to e_1 and e_2, respectively;
3. Q is the center of a hexagon of G, P_1Q and P_2Q form an angle of $\pi/3$ or $5\pi/3$;
4. any point of P_1QP_2 is either an interior or a boundary point of some hexa-

gon of G.

Definition 3 [11] A special cut segment is either an elementary cut segment or a generalized cut segment. A special edge cut E_{ij} from C_i to C_j is the set of edges of G intersected by a special cut segment form C_i to C_j. Two special edge cuts are said to be disjoint if their corresponding special cut segments are disjoint.

Definition 4 [11] A special edge cut E_{ij} is said to be of type I if $i = j$; otherwise, E_{ij} is said to be of type II.

From the definition of polyhexes, it is easy to see that a polyhex is a bipartite graph with bipartition $(B(G), W(G))$, where $B(G)$ and $W(G)$ are the set of black vertices of G and the set of white vertices of G, respectively. Thus polyhexes are 2-colorable. In the following, we make the convention that the vertices of a polyhex G in question have been colored black and white so that the end vertices of any edge have different colors. Let E be a special edge cut of G. $G - E$ is the subgraph of G obtained by deleting all the edges of E. It is evident that $G - E$ has exactly two components if E is a special edge cut of type I, and the end vertices of the edges of E have the same color when they lie in the same component of $G - E$. If E is a special edge cut of type II, then $G - E$ is still connected. Suppose that $E_{i_1 i_2}, E_{i_2 i_3}, \cdots, E_{i_r i_1}$ are r disjoint special edge cuts of type II, where $E_{i_j i_k}$ corresponds to a special cut segment from C_{i_j} to C_{i_k}, and $i_s \neq i_t$ if $s \neq t$. Let $E = E_{i_1 i_2} \cup E_{i_2 i_3} \cup \cdots \cup E_{i_r i_1}$. Then $G - E$ is disconnected and has exactly two components.

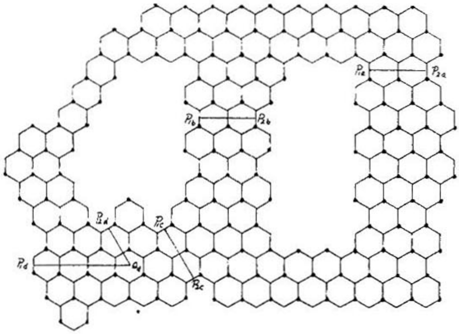

Fig.1

Definition 5 Let $E = E_{i_1i_2} \cup E_{i_2i_3} \cup \cdots \cup E_{i_ri_1}$, where $E_{i_1i_2}, E_{i_2i_3}, \cdots, E_{i_ri_1}$ are r disjoint special edge cuts of type II, $E_{i_ji_k}$ corresponds to a special cut segment from C_{i_j} to C_{i_k}, and $i_s \neq i_t$ if $s \neq t$. 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 $G - E$.

The polyhex G depicted in Fig.1 is a multiple coronoid system. Four special cut segments are given for G. Among them $P_{1d}Q_dP_{2d}$ is a generalized cut segment, and the other three special cut segments are all elementary cut segments. let E_{01} be the special edge cut corresponding to the elementary cut segment $P_{1a}P_{2a}$, E_{12} the special edge cut corresponding to the elementary cut segment $P_{1b}P_{2b}$, E_{20} the special edge cut corresponding to the elementary cut segment $P_{1c}P_{2c}$; E_{02} the special edge cut corresponding to the generalized cut segment $P_{1d}Q_dP_{2d}$. Then $E = E_{01} \cup E_{12} \cup E_{20}$ is a standard combination. While E_{02} and E_{20} do not constitute a standard combination.

Let K be a Kekulé structure of polyhex G. An edge e of G is said to be a K double bond if e belongs to K. Otherwise e is said to be a K single bond. A path L is said to be a K alternating path if the edges in L are alternately K double bond and K single bond. Similarly, a cycle D of G is said to be a K alternating cycle if the edges in D are alternately K double bond and K single bond.

Suppose that T is a subset of the vertex set $V(G)$ of G. By $\langle T \rangle$ we denote the induced subgraph of G, i.e. the subgraph of G whose vertex set is T and whose edge set is the set of those edges of G that have both end vertices in T. The neighbour set $N(T)$ of T is the set of vertices which are not in T but are adjacent to at least one vertex in T. Let G^* be a subgraph of G. Denote by $\overline{G^*} = G - G^*$ the subgraph of G obtained from G by deleting all the vertices of G^* together with their incident edges, and denote by $[G^*, \overline{G^*}]$ the set of edges each of which has one end vertex in G^* and the other in $\overline{G^*}$.

LEMMAS

Lemma 1 Let G be a Kekuléan polyhex. If G is essentially disconnected , then there is a connected subgraph G^* of G satisfying:
1. $G^* = \langle S \cup N(S) \rangle$, where S is a subset of $W(G)$ or $B(G)$ with $|S| = |N(S)|$;
2. G^* has a Kekulé structure;
3. there is at most one vertex in $N(S)$ adjacent to exactly one vertex in S.
4. all the edges of $[G^*, \overline{G^*}]$ are fixed single bonds.

Proof. Since G is essentially disconnected, G has a fixed single bond, say $e = (x, y)$. Without loss of generality, we may assume that the end vertex x is in $W(G)$. Hence the end vertex y is in $B(G)$. Let K be a kekulé structure of G. By T we denote the set of vertices to each of which there is a K alternating path starting from x and containing the fixed single bond e. We claim that vertex x is not in T. Otherwise, there is a K alternating cycle D containing the fixed single bond e, contradicting the fact that a fixed single bond can never be contained in a K alternating cycle . Let $T^* = T \cup \{y\}$, and let G^* be the subgraph induced by T^*, i.e. $G^* = \langle T^* \rangle$.

Let $S = W(G^*)$. We claim that $G^* = \langle S \cup N(S) \rangle$. It suffices to prove that $N(S) = B(G^*)$. For each vertex u in $N(S)$, u is adjacent by an edge, say e^*, to a vertex v in S. By the definition of S, there is a K alternating path P from x to v containing e. It is not difficult to see that the last edge in P is a K double bond. Hence e^* is a K single bond. Therefore, there is a K alternating path $P' = P \cup \{e^*\}$ from x to u containing e, which implies that u is in G^*. As v is in $W(G^*)$, u is in $B(G^*)$. We have proved that $N(S) \subseteq B(G^*)$. For a vertex $w \neq y$ in $B(G^*)$, by the definition of G^*, there is a K alternating path P from x to w containing e. Thus the white vertex on P which is adjacent to w is in $W(G^*) = S$. Hence w is in $N(S)$ which implies that $B(G^*) \subseteq N(S)$. Consequently, $N(S) = B(G^*)$. From the definition of G^*, it is not difficult to see that G^* is connected. Moreover, one can see that G^* has a Kekulé structure $K^* = K \cap G^*$. Hence $|S| = |W(G^*)| = |B(G^*)| = |N(S)|$.

Let h ($h \neq y$) be a vertex in $N(S)$. We claim that h is adjacent to at least two vertices in S. From the definition of G^* there is a K alternating path $P = xy \cdots\cdots x_p h$ from x to h. One can check that the last edge (x_p, h) is a K single bond since h is a black vertex. As G^* has a Kekulé structure, h is saturated by a K double bond (h, f). Hence there is a K alternating path $P' = xy \cdots x_p hf$ from x to f. This implies that the vertex f is in S. Therefore, h is adjacent to at least two vertices in S, i.e. x_p and f . Consequently, the vertex y is the only possible vertex in $N(S)$ which is adjacent to exactly one vertex in S.

Note that for any Kekulé structure of G^*, the vertices of S are saturated only by the vertices of $N(S)$. Since $|S| = |N(S)|$, none of the vertices of $N(S)$ can match the vertices of $\overline{G^*}$. Therefore, all the edges of $[G^*, \overline{G^*}]$ are fixed single bonds.

Lemma 2 An essentially disconnected polyhex G has at least one fixed single bond on the boundary of G.

Proof. We use the notations introduced above. By Lemma 1, G has a connected Kekuléan subgraph G^* such that all the edges of $[G^*, \overline{G^*}]$ are fixed single bonds, where $\overline{G^*} = G - G^*$. In order to separate G^* from $\overline{G^*}$, we use a Jordan curve J, i.e. a closed non-self-intersected curve in the plane. We make the convention that J intersects each edge in $[G^*, \overline{G^*}]$ at the midpoint of the edge, and the segments of J within G is either a line segment or a broken line segment,;

and if J passes a hexagon of G, it must pass its center; and if J turns within a hexagon of G, it must turn at the center of the hexagon. Since $G^* = \langle S \cup N(S) \rangle$ with S being a subset of $W(G)$, the end vertices of edges in $[G^*, \overline{G^*}]$ are of black when they lie in G^* , and the end vertices of edges in $[G^*, \overline{G^*}]$ are of white when they lie in $\overline{G^*}$. Thus at each turning point of J the angle is $\pi/3$ or $5\pi/3$. Note that all the edges of $[G^*, \overline{G^*}]$ are fixed single bonds. There cannot be two consecutive turning points with the same angle $\pi/3$ or $5\pi/3$. Otherwise, no matter whether the vertices within the angle of $\pi/3$ belong to G^* or $\overline{G^*}$, a vertex within the angle of $\pi/3$ cannot be saturated by a K double bond , contradicting that G is Kekuléan. Bear in mind that at each turning point of J if the vertices within the angle of $\pi/3$ belong to G^*, then there is a vertex in $N(S)$ which is adjacent to exactly one vertex in S. By the construction of G^*, vertex y is the only possible vertex which is adjacent to exactly one vertex in S. Therefore, there are at most one angle of $\pi/3$ facing the interior of G^*, and the total number of turning points is at most three. Consequently, each segment of J within G can only be one of the following four modes: 1. a line segment without turning point; 2. a broken line segment which has exactly one turning point with angle $\pi/3$ or $5\pi/3$; 3. a broken line segment which has two turning points, one with angle $\pi/3$ and the other with angle $5\pi/3$; 4. a broken line segment which has three turning points, the order of angles is: $5\pi/3$, $\pi/3$ and $5\pi/3$. One can check that in each case, the segment of J within G cannot be closed. Therefore, J must meet some boundary of G. This implies that there must be some fixed single bonds of $[G^*, \overline{G^*}]$ lying on some boundary of G.

Lemma 3 Let G be a Kekuléan polyhex. If G possesses a special edge cut E of type I, or a standard combination E such that $|B(G_i)| = |W(G_i)|$ for the two components $G_i (i = 1, 2)$ of $G - E$, then G is essentially disconnected.
Proof. Since E is a special edge cut of type I, or a standard combination, the end vertices of the edges in E have the same color when they lie in the same component of $G - E$. Without loss of generality, we may assume that the end vertices of the edges in E are black when they lie in G_1. Denote by S the set of white vertices of G_1, i.e. $S = W(G_1)$. Then the set of black vertices of G_1 is $N(S)$, i.e. $N(S) = B(G_1)$. Hence $G_1 = \langle S \cup N(S) \rangle$. It is evident that in any Kekulé structure of G, the vertices in S can only be matched by the vertices in $N(S)$. By the condition $|B(G_1)| = |W(G_1)|$, we have $|S| = |N(S)|$. This means that none of the vertices of $N(S)$ can match the vertices of G_2. Therefore, none of the edges in E belongs to any Kekulé structure of G, which implies that all the edges in E are fixed single bonds. Consequently, G is essentially disconnected.

Now we are in the position to formulate our main result.
Theorem Let G be a Kekuléan polyhex, C_0 the boundary of G; $C_1, C_2, \cdots, C_m$

the inner boundaries of G (if any). Then G is essentially disconnected if and only if G possesses a special edge cut E of type I, or a standard combination E such that $|B(G_i)| = |W(G_i)|$ for the two components $G_i(i = 1, 2)$ of $G - E$.
Proof. Sufficiency follows immediately from Lemma 3.
Necessity. Suppose that G is essentially disconnected. Then G has a fixed single bond, say $e_1 = (x, y)$, lying on some of the boundaries of G (Lemma 2). Without loss of generality, we may assume that the end vertex x is in $W(G)$. Hence the end vertex y is in $B(G)$. Let K be a Kekulé structure of G. By T we denote the set of vertices to each of which there is a K alternating path starting from x and containing the fixed single bond e_1. Let $T^* = T \cup \{y\}$, and let G^* be the subgraph induced by T^*, i.e. $G^* = \langle T^* \rangle$. From the proof of Lemma 1, one can see that G^* is connected and satisfies: 1. $G^* = \langle S \cup N(S) \rangle$, where $S = W(G^*)$ and $N(S) = B(G^*)$ with $|S| = |N(S)|$; 2. $K^* = K \cap G^*$ is a Kekulé structure of G^*; 3. vertex y is the only possible vertex in $N(S)$ which is adjacent to exactly one vertex in S; 4. all the edges of $[G^*, \overline{G^*}]$ are fixed single bonds.

Now we use a Jordan curve J to separate G^* from $\overline{G^*}$. As before, We make the convention that J intersects each edge in $[G^*, \overline{G^*}]$ at the midpoint of the edge, and the segments of J within G is either a line segment or a broken line segment; and if J passes a hexagon of G, it must pass its center; and if J turns within a hexagon of G, it must turn at the center of the hexagon. Suppose that the edges in $[G^*, \overline{G^*}]$ are met by J in the cyclic order: $e_1, e_2, \cdots, e_{p_1}; e_{p_1+1}, \cdots, e_{p_2}; \cdots\cdots; e_{p_{q-2}+1}, \cdots, e_{p_{q-1}}; e_{p_{q-1}+1}, \cdots, e_{p_q}$; where e_{p_i} and e_{p_i+1} are on C_{u_i} for $i = 1, 2, \cdots, q-1$; e_1 and e_{p_q} are on C_{u_q}; where $\{u_1, u_2, \cdots\cdots, u_q\} \subseteq \{1, 2, \cdots\cdots, m\}$; e_j is not on any boundary of G when $j \neq 1, p_1, p_1+1, p_2, \cdots\cdots, p_{q-2}+1, p_{q-1}, p_{q-1}+1, p_q$. Let $E_r = \{e_{p_{r-1}+1}, e_{p_{r-1}+2}, \cdots, e_{p_r}\}(r = 1, 2, \cdots, q)$, here we make the convention that $p_0 = 0$. Denote by J_r the segment of J intersecting the edges of E_r, i.e. the segment between the midpoint of $e_{p_{r-1}+1}$ and the midpoint of e_{p_r}.

We distinguish two cases:
Case 1: G is a benzenoid system. Then G has exactly one boundary C_0. Therefore, $q = 1$, e_1 and e_{p_1} are on C_0. As indicated in the proof of Lemma 2, J_1 can only be one of the following four modes: 1. a line segment without turning point; 2. a broken line segment which has exactly one turning point with angle $\pi/3$ or $5\pi/3$; 3. a broken line segment which has two turning points, one with angle $\pi/3$ and the other with angle $5\pi/3$; 4. a broken line segment which has three turning points, the order of angles is: $5\pi/3$, $\pi/3$ and $5\pi/3$. Note that e_1 lies on C_0. One can check that J_1 cannot be of mode 4. If J_1 is of mode 1 or mode 2, then J_1 is already a special cut segment from C_0 to C_0. This means that $E = E_1$ is a special edge cut of type I. Since all the edges in E are fixed single bonds, each component of $G - E$ has a Kekulé structure. Hence we have $|B(G_i)| = |W(G_i)|$ for the two components $G_i(i = 1, 2)$ of $G - E$. Now suppose

that J_1 is of mode 3. Since all the edges intersected by J_1 are fixed single bonds, we find a series of fixed double bonds (indicated by double lines in Fig.2). Shift Q_1Q_2 to $Q_1'Q_2'$. If $Q_1'Q_2'$ does not intersect C_0, then replace E_1 by E_1' which corresponds to the generalized cut segment $Q_1'Q_2'P_2$. Then E_1' is a special edge cut of type I consisting of fixed single bonds such that $|B(G_i)| = |W(G_i)|$ for the two components $G_i (i = 1, 2)$ of $G - E_1'$. If $Q_1'Q_2'$ intersects C_0, then we can find at least a special edge cut E' (cf.Fig.2) consisting of fixed single bonds such that $|B(G_i)| = |W(G_i)|$ for the two components $G_i (i = 1, 2)$ of $G - E'$.

Fig.2

Case 2: G is a coronoid system. For $r = 1, 2, \cdots, q$, J_r is one of the four modes as indicated in the proof of Lemma 2. Bear in mind that at each turning point of J if the vertices within the angle of $\pi/3$ belong to G^*, then there is a vertex in $N(S)$ which is adjacent to exactly one vertex in S. Note that vertex y is the only possible vertex which is adjacent to exactly one vertex in S, and y is on boundary C_{u_q}. One can check that $J_2, J_3, \cdots, J_q$ must be an elementary cut segment or a generalized cut segment with turning angle being $5\pi/3$. Now consider J_1. By a similar reasoning as above, J_1 can not be of mode 4. If J_1 is of mode 1 or mode 2, then J_1 is already an elementary cut segment or a generalized cut segment. This means that E_1 is a special edge cut of type II. One can check that $E = E_1 \cup E_2 \cup \cdots \cup E_q$ is a standard combination such that $|B(G_i)| = |W(G_i)|$ for the two components $G_i (i = 1, 2)$ of $G - E$. Now suppose that J_1 is of mode 3. In a similar way as in case 1, we find a series of fixed double bonds (indicated by double lines in Fig.3). Shift Q_1Q_2 to $Q_1'Q_2'$. If $Q_1'Q_2'$

does not intersect any boundary of G, then replace E_1 by E_1' which corresponds to the generalized cut segment $Q_1'Q_2'P_2$. Then $E' = E_1' \cup E_2 \cup \cdots \cup E_q$ is a

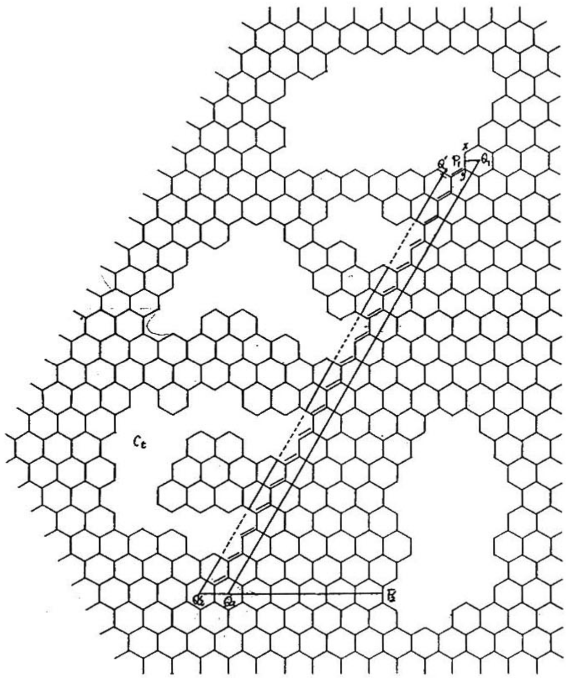

Fig.3

standard combination such that $|B(G_i)| = |W(G_i)|$ for the two components $G_i(i = 1, 2)$ of $G - E'$. If $Q_1'Q_2'$ intersects some boundary C_t more than two times, then we can find a special edge cut E' of type I corresponding to an elementary cut segment (see Fig.3). One can check that E' consists of fixed single bonds such that $|B(G_i)| = |W(G_i)|$ for the two components $G_i(i = 1, 2)$ of $G - E'$. Now we consider the case that $Q_1'Q_2'$ intersects some boundaries of $G : C_{d_1}, C_{d_2}, \cdots, C_{d_p} (p \geq 1)$, and $Q_1'Q_2'$ intersects each of them exactly two times (cf. Fig.3). If none of $C_{d_1}, C_{d_2}, \cdots, C_{d_p}$ belongs to $\{C_{u_1}, C_{u_2}, \cdots, C_{u_q}\}$, then we replace E_1 by a series of special edge cuts E_{11}, E_{12}, $\cdots$, E_{1h} each of them corresponds to an elementary cut segment, together with a special edge cut $E_{1,h+1}$ which corresponds to a g-cut segment. Let $E' = (E_{11} \cup E_{12} \cup \cdots \cup E_{1h} \cup E_{1,h+1}) \cup E_2 \cup \cdots \cup E_q$. One can check that E' is a standard combination such that $|B(G_i)| = |W(G_i)|$ for the two components $G_i (i = 1, 2)$ of $G - E'$. If some of $C_{d_1}, C_{d_2}, \cdots, C_{d_p}$ belongs to $\{C_{u_1}, C_{u_2}, \cdots, C_{u_q}\}$, let $t (1 \leq t \leq p)$ be the smallest natural number such that C_{d_t} is among $C_{u_1}, C_{u_2}, \cdots, C_{u_q}$. Suppose that $C_{d_t} = C_{u_j}$. We replace E_1 by a series of special edge cuts E_{11}', E_{12}', $\cdots$, E_{1t}' (cf. Fig.4). One can check that $E' = (E_{11}' \cup E_{12}' \cup \cdots \cup E_{1t}') \cup E_{j+1} \cup E_{j+2} \cup \cdots \cup E_q$ is a standard combination such that $|B(G_i)| = |W(G_i)|$ for the two components $G_i (i = 1, 2)$ of $G - E'$.

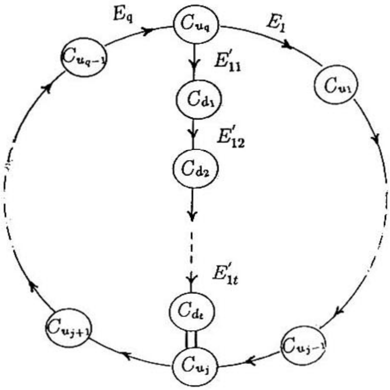

Fig.4

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