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A NECESSARY AND SUFFICIENT CONDITION FOR THE EXISTENCE OF KEKULÉ STRUCTURES IN BENZENOID SYSTEMS

Rong-qin Sheng

Shanghai Institute of Computer Technology,
546 Yu Yuan Road, Shanghai,
The People's Republic of China

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ABSTRACT

A necessary and sufficient condition for the existence of Kekulé structures in benzenoid systems is developed, which is stronger than that of Kostochka[2].

1. INTRODUCTION

The problem of the existence of Kekulé structures in benzenoid systems has been investigated for a long time. A number of new discoveries have been made in the last few years. Two fast algorithms for recognizing Kekuléan benzenoid systems have been reported[3,4].

In 1985 two necessary and sufficient structural requirments for the existence of Kekulé structures in benzenoid systems were discovered by Zhang, Chen and Guo[1] and Kostochka[2]. The two results are quite similar. Kostochka's result is somewhat stronger.

In the present paper, A stronger result than that of Kostochka[2] will be described.

2. ELEMENTARY EDGE-CUTS AND K-EDGE-CUTS

Benzenoid systems are defined in the usual way[5,6]. The vertices and edges lying on the perimeter are called external, otherwise internal. Benzenoid systems are bipartite: their vertices can be colored by two colors (say white and black), so that vertices of same color are never adjacent. Denote by $n^{(w)}(G)$ and $n^{(b)}(G)$ respectively the numbers of white and black vertices in a colored bipartite graph G. Furthermore,

$$D(G) = n^{(b)}(G) - n^{(w)}(G). \qquad (1)$$

Then a well known necessary condition for a benzenoid system B to be Kekulean is

$$D(B) = 0. \qquad (2)$$

Benzenoid systems for which (2) is violated are said to be obvious non-Kekuléan. The non-Kekuléan benzenoid systems for which (2) is realized are called concealed non-Kekuléan.

An edge-cut[1] of B is a collection of edges C such that the subgraph B-C obtained from B by deleting all edges in C has more components than B.

An elementary edge-cut (EEC) is a collection of all edges intersected by a straight line segment P_1P_2 which satisfies:

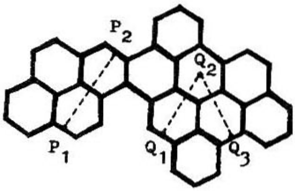

Fig. 1

(i) P_1P_2 orthogonally intersects a number of mutually parallel edges,

(ii) each of P_1, P_2 is the center of an external edge,

(iii) every point of P_1P_2 is either an interior or a boundary point of some hexagon of B,

(iv) the subgraph obtained from B by deleting all edges intersected by P_1P_2 has exactly two components (see Fig. 1).

A K-edge-cut (KEC) is a collection of all edges intersected by a broken line segment $Q_1Q_2Q_3$ which satisfies:

(i) each of Q_1Q_2, Q_2Q_3 orthogonally intersects a number of mutually parallel edges,

(ii) $\angle Q_1Q_2Q_3 = 60^\circ$,

(iii) each of Q_1, Q_3 is the center of an external edge,

(iv) the angular point Q_2 is the center of an hexagon of B,

(v) every point of $Q_1Q_2Q_3$ is either an interior or a boundary point of some hexagon of B,

(vi) the subgraph obtained from B by deleting all edges intersected by $Q_1Q_2Q_3$ has exactly two components (see Fig. 1).

Let C be an EEC or a KEC of B. Then B-C has two components B', B". If B is colored, then one component contains the black end vertices of all edges in C, this component is defined as B' (therefore B" contains the white end vertices of all edges in C).

Kostochka[2] put forward a necessary and sufficient condition that A benzenoid system B is Kekuléan if and only if

(i) $D(B) = 0$, (ii) for every EEC and every KEC,

$$D(B') \geqslant 0. \qquad (3)$$

Let B be a benzenoid system with $D(B) = 0$. C is an EEC or a KEC. Then $D(B') = -D(B")$. (4)

Sometimes the value $D(B')$ is also symbolized as $D(C)$:

$$D(C) = D(B'). \qquad (5)$$

We have simple ways to calculate $D(B)$ and $D(B')$:

If B is oriented with some of its edges vertical, and the peaks are black, then $D(B)$ is equal to the difference between the numbers of peaks and valleys in B.

Let C_E be an EEC. we may assume the edges of C_E are vertical.

Denote by s the difference between the numbers of peaks and valleys in the upper component. The number of edges in C_E is denoted by tr. Then $D(B') = D(C_E) = tr-s$.

Let C_K be a KEC. B is oriented with some of its edges vertical. We may assume any edge of C_K is not vertical. Then $D(B')$ (or $D(C_K)$) is equal to the difference between the numbers of peaks and valleys in the upper component.

3. A NECESSARY AND SUFFICIENT CONDITION

A characteristic K-edge-cut (CKEC) is defined as a KEC in which the four end vertices of the two external edges are all of degree three. Fig. 2 depicts an example.

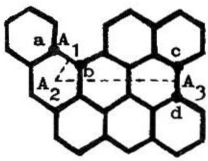

Fig. 2. A KEC realized by $A_1A_2A_3$ is a CKEC because a,b,c,d are all of degree three.

In a benzenoid system, the CKECs only have a small part in the KECs. Actually there are a great number of benzenoid systems which have no CKECs. Fig. 3 shows two examples.

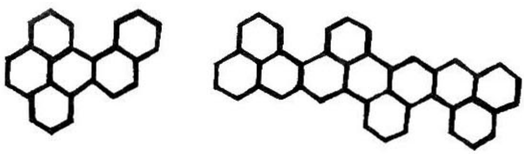

Fig. 3. Two benzenoid systems which have no CKECs.

The following theorem shows a necessary and sufficient structural requirement for the existence of Kekulé structures in benzenoid systems.

THEOREM. A benzenoid system B is Kekuléan if and only if (i) D(B) = 0, (ii) for every EEC and every CKEC, $D(B') \geqslant 0$.

The theorem is derived from Kostocha's result and the following lemma.

LEMMA. If B is a concealed non-Kekuléan benzenoid system, and the relation (3) is realized for every EEC, then B has a CKEC for which (3) is violated.

Proof. Let B be oriented with some of its edges vertical and contain the hexagons of side length 1. Because B is concealed non-Kekuléan and (3) is realized for every EEC, according to Kostochka's result B has a KEC for which (3) is violated. We may assume this KEC satisfies:

(a) any edge in the KEC is not vertical,

(b) the highest point of its corresponding broken line segment is the angular point.

All KECs satisfying (a) and (b) constitute a set **Z**.

$$\text{Let}\quad Z^* = \left\{ C' \;\middle|\; D(C') = \min_{C \in Z} D(C),\ C' \in Z \right\}. \qquad (6)$$

Choose a KEC C^* which is realized by $R_1R_2R_3$ and satisfies:

(c) $C^* \in Z^*$,

(d) for any KEC in Z^* realized by $Q_1Q_2Q_3$, R_2 is not below Q_2.

Obviously C^* is a KEC for which (3) is violated. We shall verify that C^* is a CKEC.

We may assume that $B-C^*$ has the upper component B' and the lower component B".

See Fig. 4, C^* has two external edges: $\{u,v\}$, $\{x,y\}$, R_2' and R_2'' are two points of the straight line through R_2, R_3

such that $R_2'R_2$ and R_2R_2'' are of length $\sqrt{3}$, R_2' lies above R_2''. Then each of R_2', R_2'' is either the center of a hexagon of B or outside any hexagon of B.

Denote by $\mathbf{E}(L)$ the set of all edges intersected by the line L. Let

Y'= the set of all edges which belong to B' and share incident edges with the edges in $E(R_1R_2)$,

Y"= the set of all edges which belong to B" and share incident edges with the edges in $E(R_1R_2)$.

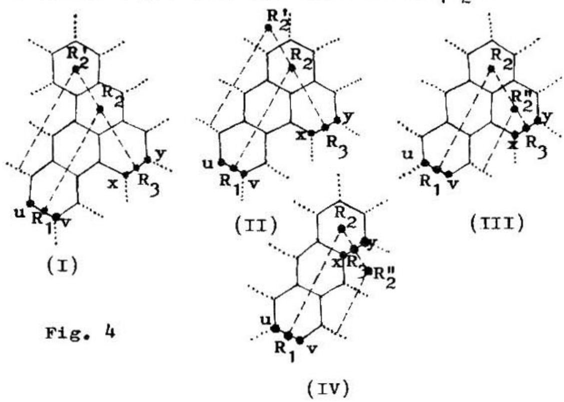

Fig. 4

Intuitively, Y' (Y") is a set of the edges intersected by a straight line segment through R_2' (R_2'') and parallel to R_1R_2.

If it is not realized that u and v are of degree three, then there are four possible cases:

(I) u is of degree two and R_2' is the center of a hexagon of B (see Fig. 4I). Then $Y' \cup E(R_2'R_3)$ is composed of t ($t \geqslant 0$) EECs C_1, C_2, ..., C_t and one KEC C_1^*. It follows that

$$\sum_{i=1}^{t} D(C_i) + D(C_1^*) = D(C^*).$$

Thus $D(C_1^*) \leqq D(C^*)$.

By (6) and (c), $C_1^* \in Z^*$, which contradicts (d) because C_1^* is realized by a broken line segment with angular point R_2' lying above R_2.

(II) u is of degree two and R_2' is outside any hexagon of B (see Fig. 4II). Then $Y' \cup E(R_2'R_3)$ is composed of t $(t \geqslant 1)$ EECs $C_1, C_2, \ldots, C_t$. It follows that

$$\sum_{i=1}^{t} D(C_i) = D(C^*) < 0,$$ which is a contradiction.

(III) v is of degree two and R_2'' is the center of a hexagon of B (see Fig. 4III). Then $Y'' \cup E(R_2''R_3)$ is composed of t $(t \geqslant 0)$ EECs $C_1, C_2, \ldots, C_t$ and one KEC C_2^*. It follows that

$$\sum_{i=1}^{t} D(C_i) + D(C_2^*) = D(C^*) - 1.$$

Thus $D(C_2^*) < D(C^*)$, which contradicts (c) and (6) because $C_2^* \in Z$.

(IV) v is of degree two and R_2'' is outside any hexagon of B (see Fig. 4IV). Then Y'' is composed of t $(t \geqslant 0)$ EECs $C_1, C_2, \ldots, C_t$. It follows that

$$\sum_{i=1}^{t} D(C_i) = D(C^*) - 1 < 0,$$ which is a contradiction.

Consequently, u and v are of degree three. By the similar proof, x and y are also of degree three. Hence C^* is a CKEC. The proof is completed.

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