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ON THE EXISTENCE OF KEKULÉ STRUCTURES IN BENZENOID SYSTEMS

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ABSTRACT

A simple necessary and sufficient condition is obtained for the existence of Kekulé structures in benzenoid systems. It is stronger than the previous one given in Ref.1 and can be recommended as an easy way to recognize Kekuléan benzenoid systems.

1. Introduction

The existence of Kekulé structures in benzenoid systems was considered one of the most difficult problems in the theory of benzenoid hydrocarbons. Much progress in this topic, including two fast algorithms[2,3], has been made in the past few years.

In 1985 two similar necessary and sufficient structural requirements were discovered by Zhang, Chen and Guo[4] and Kostochka[5], and Kostochka's result is somewhat stronger. Recently, the present author[1] put forward a substantial improvement of Kostochka's work[5]. In the present paper, a stronger result than the previous one[1] is obtained, and it seems to be a simple criterion of recognizing the Kekuléan/non-Kekuléan nature of benzenoid systems.

2. Edge-cuts

A benzenoid system is said to be Kekuléan if it possesses a Kekulé structure (i.e. 1-factor), otherwise it is non-Kekuléan. The vertices and edges belonging to the perimeter are called external, otherwise internal.

Benzenoid systems are bipartite: their vertices can be colored by two colors (say white and black) such that vertices of same color are never adjacent.

Let $n^{(w)}(G)$ and $n^{(b)}(G)$ denote the numbers of white and black vertices in a colored bipartite graph G, respectively. Furthermore, $D(G) = n^{(b)}(G) - n^{(w)}(G)$. (1)

A well known necessary condition for a benzenoid system B to be Kekuléan is $D(B) = 0$. (2)

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

Let B be a benzenoid system and $e_1, e_2, \ldots, e_t$ some of its edges. Then $C = \{e_1, e_2, \ldots, e_t\}$ is called an edge-cut of B if

(a) by deleting the edges $e_1, e_2, \ldots, e_t$ from B it decomposes into two parts B' and B";

(b) the black end vertex of e_i belongs to B' (and therefore the white end vertex of e_i belongs to B"), $i=1,2,\ldots,t$;

(c) each pair of edges e_i, e_{i+1}, $i=1,2,\ldots,t-1$, belongs to the same hexagon and e_1 and e_t belongs to the perimeter.

An elementary edge-cut (EEC) is an edge-cut realized by a straight line segment (see Fig. 1).

A K-edge-cut (KEC) is an edge-cut realized by a broken line segment consisting of two straight line segments which form an angle of 60° (see Fig. 1) and intersect the perimeter only twice.

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 (see Fig. 1).

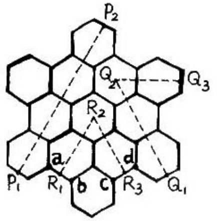

Fig. 1. The set of edges intersected by P_1P_2 is an EEC, the set of edges intersected by $Q_1Q_2Q_3$ is a KEC, and the set of edges intersected by $R_1R_2R_3$ is a CKEC because a, b, c and d are all of degree three.

THEOREM 1 (Kostochka[5]). A benzenoid system B is Kekuléan if and only if (i) D(B)=0; (ii) for every EEC and KEC, $D(B') \geqslant 0$.

THEOREM 2 (Sheng[1]). A benzenoid system B is Kekuléan if and only if (i) D(B)=0; (ii) for every EEC and CKEC, $D(B') \geqslant 0$.

Let C be an edge-cut of B. Sometimes the value D(B') is also symbolized as D(C): $D(C) = D(B')$. (3)

3. A Simple Necessary and Sufficient Condition

A characteristic elementary edge-cut (CEEC) is defined as an EEC in which at least three end vertices of the two external edges are of degree three (Fig. 2).

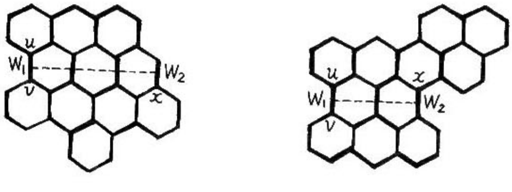

Fig. 2. The set of edges intersected by W_1W_2 is a CEEC because u, v and x are of degree three.

The following is a stronger result than Theorem 2.

THEOREM 3. A benzenoid system B is Kekuléan if and only if (i) $D(B)=0$; (ii) for every CEEC and CKEC, $D(B')\geqslant 0$.

Proof. The necessity is obvious, and we need only to verify the sufficiency. Let B be a benzenoid system satisfying:

(d) $D(B)=0$;

(e) for every CEEC and CKEC, $D(B')\geqslant 0$.

We shall prove that B is Kekuléan.

Suppose that B is non-Kekuléan. From (d), B is concealed non-Kekuléan. According to (d), (e) and Theorem 2, B must possess an EEC for which $D(B')<0$. Since B is finite, we can select an EEC C^* satisfying:

(f) $D(C^*)<0$;

(g) $B-C^*$ has two components $B'(C^*)$ and $B''(C^*)$;

(h) for every EEC of B belonging to $B'(C^*)$, $D(B')\geqslant 0$.

We may orient B such that the edges of C^* are vertical and $B'(C^*)$ is the upper component of $B-C^*$. Also, we may assume the edges of B are of length 1. Let $\{u,v\}$ and $\{x,y\}$ be the two external edges of C^*, where u and x lie above v and y. Then, both u and x must be of degree three. Otherwise, without loss of generality, we may assume x is of degree two, make a path lying on the perimeter of B: $u_0=u$, $u_1,u_2,\ldots,u_t$, where $u_1\neq v$, $\{u_{t-1},u_t\}$ is vertical and $\{u_{i-1},u_i\}$ is non-vertical for $i=1,2,\ldots,t-1$, and conclude contradictions in the following two possible cases.

Case 1. u_t lies above u (Fig. 3). In this case, it must

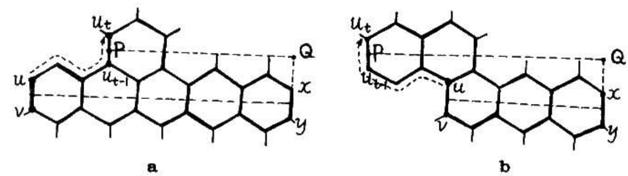

Fig. 3

follow $t \geq 2$, and t must be an even number. Let P be the center of $\{u_{t-1}, u_t\}$, and extend yx to Q such that xQ is of length 1. Let $E(L)$ denote the set of edges of B intersected by L. Then $E(PQ)$ is composed of k ($k \geq 1$) EECs: $C_1, C_2, \ldots, C_k$, belonging to $B'(C^*)$ and satisfying

$$\sum_{i=1}^{k} D(C_i) = \begin{cases} D(C^*)-1, & \text{if } u \text{ is of degree two (Fig. 3a);} \\ D(C^*), & \text{if } u \text{ is of degree three (Fig. 3b).} \end{cases}$$

Thus $\sum_{i=1}^{k} D(C_i) < 0$, which contradicts (h).

Case 2. u_t lies below u (Fig. 4). In this case, it must hold $t \geq 3$, and t must be an odd number. Both u_{t-2} and u_{t-1} must be of degree three. Let R be the center of $\{u_{t-2}, u_{t-1}\}$ and S_1 the center of the hexagon containing $\{u_{t-2}, u_{t-1}\}$. The straight line through R and S_1 intersects m ($m \geq 1$) hexagons whose centers are $S_1, S_2, \ldots, S_m$. S_{m+1} lies on this line and outside any hexagon of B such that $S_m S_{m+1}$ is of length $\sqrt{3}$. Extend yx to W_1 such that xW_1 is

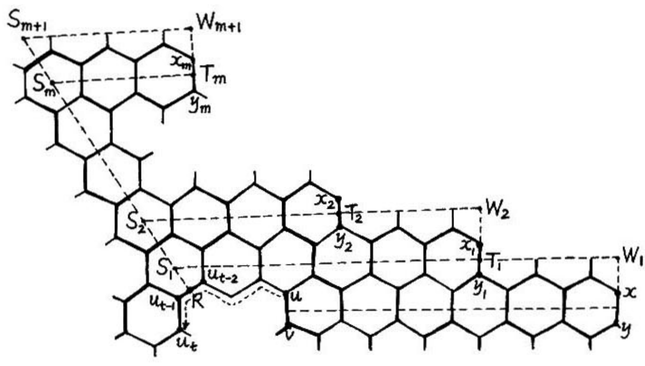

Fig. 4

of length 1. Then $E(RS_1W_1)$ is composed of one KEC C_1^* and t_1 $(t_1 \geqslant 0)$ EECs: $C_1^{(1)}, C_2^{(1)}, \ldots, C_{t_1}^{(1)}$, belonging to $B'(C^*)$ and satisfying

$$D(C_1^*) + \sum_{i=1}^{t_1} D(C_i^{(1)}) = D(C^*) < 0.$$

By (h), $D(C_1^*) < 0$. Obviously, $C_1^* = E(RS_1T_1)$, where T_1 is the center of $\{x_1, y_1\}$, the vertical external edge of C_1^*, and x_1 lies above y_1. From (e), C_1^* is not a CKEC, hence x_1 must be of degree two. If $m \geqslant 2$, extend y_1x_1 to W_2 such that x_1W_2 is of length 1. Then $E(RS_2W_2)$ is composed of one KEC C_2^* and t_2 $(t_2 \geqslant 0)$ EECs: $C_1^{(2)}, C_2^{(2)}, \ldots, C_{t_2}^{(2)}$, belonging to $B'(C^*)$ and satisfying

$$D(C_2^*) + \sum_{i=1}^{t_2} D(C_i^{(2)}) = D(C_1^*) < 0.$$

By (h), $D(C_2^*) < 0$. Obviously, $C_2^* = E(RS_2T_2)$, where T_2 is the center of $\{x_2, y_2\}$, the vertical external edge of C_2^*, and x_2 lies above y_2. From (e), C_2^* is not a CKEC, hence x_2 must be of degree two. This process continues if $m \geqslant 3$, and we can eventually get the KEC $C_m^* = E(RS_mT_m)$ satisfying $D(C_m^*) < 0$, where T_m is the center of $\{x_m, y_m\}$, the vertical external edge of C_m^*, and x_m lies above y_m and is of degree two. Extend y_mx_m to W_{m+1} such that x_mW_{m+1} is of length 1. Then $E(RS_{m+1}W_{m+1})$ is composed of t_{m+1} $(t_{m+1} \geqslant 1$ because $E(RS_{m+1})$ is an EEC.) EECs: $C_1, C_2, \ldots, C_{t_{m+1}}$, belonging to $B'(C^*)$ and satisfying

$$\sum_{i=1}^{t_{m+1}} D(C_i) = D(C_m^*) < 0,$$

which contradicts (h).

Now, we have proved that both u and x are of degree three. According to (e), C^* is not a CEEC, therefore both v and y are of degree two. Hence C^* satisfies

(I) the two upper end vertices of the two external edges are of degree three;

(II) the two lower end vertices of the two external edges are of degree two. Extend uv and xy to R_1 and R_2 respectively such that vR_1 and yR_2 are of length 1 (Fig. 5). Then $E(R_1R_2)$ is composed of s $(s \geq 1)$ EECs:

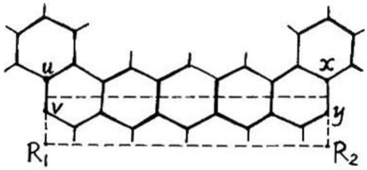

Fig. 5

$C^1, C^2, \ldots, C^s$, satisfying (I) and

$\sum_{i=1}^{s} D(C^i) = D(C^*)-1 < 0$. Thus, there exists an EEC C^k $(1 \leq k \leq s)$ satisfying $D(C^k) < 0$. According to (e), C^k is not a CEEC, hence C^k also satisfies (II). Now, we obtain a statement that for an arbitrary EEC C_E satisfying (I), (II) and $D(C_E) < 0$, there exists another EEC C'_E satisfying (I), (II) and $D(C'_E) < 0$, and the edges of C'_E lie below these of C_E. Since B is finite, it can not possess an EEC satisfying (I), (II) and $D(B') < 0$, which is a contradiction because C^* is such an EEC.

Consequently, B must be Kekuléan. The proof is completed.

Theorem 3 provides a simple way to determine whether or not a given benzenoid system possesses a Kekulé structure. In particular, if B possesses no CEEC and CKEC, then $D(B)=0$ becomes the necessary and sufficient condition for B to be Kekuléan. Fig. 6 depicts two examples of Kekuléan

Fig. 6

benzenoid systems with no CEEC and CKEC.

An algorithm is thus derived from Theorem 3. Let B be a benzenoid system. We first calculate D(B). If D(B) $\neq$ 0, then B is non-Kekuléan. If D(B) = 0, we calculate D(B') for CEECs and CKECs: if there exists a CEEC or a CKEC for which D(B') $<$ 0, then B is non-Kekuléan; if D(B') $\geqslant$ 0 for every CEEC and CKEC, then B is Kekuléan. Two examples are depicted in Fig. 7.

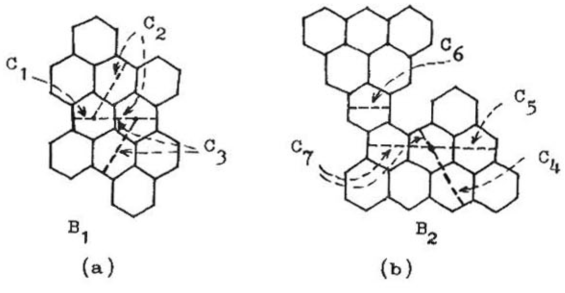

Fig. 7. (a) B_1 possesses one CEEC C_1 and two CKECs C_2,C_3. Since $D(B_1)=0$, $D(C_1)=D(C_2)=D(C_3)=1$, B_1 is Kekuléan. (b) B_2 possesses three CEECs C_4,C_5,C_6 and one CKEC C_7. B_2 is non-Kekuléan because $D(C_6)=-1 < 0$ or $D(C_7)=-1 < 0$.

We have simple ways to calculate D(B) and D(B'), which were introduced in Ref.1 and are now reviewed in the following.

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 orient B so that the edges of C_E are vertical. Let s designate 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. We may orient B so that some of its edges are vertical and 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.

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