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RECOGNITION OF ESSENTIALLY DISCONNECTED BENZENOIDS

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Dedicated to the memory of the late
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Abstract: Essentially disconnected benzenoids are Kekuléan pericondensed benzenoids with some fixed bonds. A necessary and sufficient condition for a Kekuléan benzenoid to be essentially disconnected is given and rigorously proved. The concept of standard horizontal cut is introduced. Smallest essentially disconnected benzenoids with some characteristics are given and proved to be unique. A simple criterion for essentially disconnected benzenoids with h (the number of hexagons) ≤ 14 is reported.

INTRODUCTION AND DEFINITIONS

The term "essentially disconnected benzenoid" was used for the first time by Cyvin et al.[1] to indicate a Kekuléan (pericondensed) benzenoid with fixed bonds. But, of course, the existence of such systems has been known long before that. Here a benzenoid is defined in the usual way.[2,3] The concept does not include coronoids[4] or generalized benzenoids.[5]

An essentially disconnected benzenoid consists of two kinds of parts: effective units and junction. The effective units are normal benzenoids, i.e. Kekuléan benzenoids without fixed bonds; the junction may be a benzenoid or a coronoid, or may be separated into two or more benzenoids or coronoids (see Fig. 1).

Essentially disconnected benzenoids have proved to be very useful in

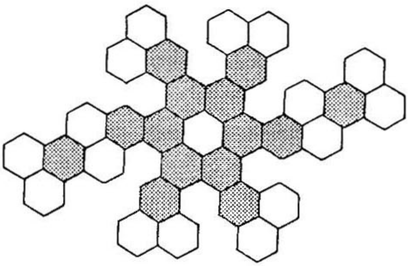


Fig. 1. An essentially disconnected benzenoid with 9 effective units. The junction (grey) consists of one quasi-coronoid, viz. hexabenzo[6]circulene and two benzenoids (benzenes).

certain enumeration techniques for Kekulé structures.[6] Several papers concerning essentially disconnected benzenoids have appeared.[1,7-10] The recognition of essentially disconnected benzenoids seems to be a most important task when dealing with this kind of benzenoids. Cyvin and Gutman[8] discovered two sufficient conditions for a Kekuléan benzenoid to be essentially disconnected. But neither of them are necessary.[9] A necessary and sufficient condition was found as a by-product of recent studies.[12] However, it is not convenient to be used in practice. In the present work we give a better necessary and sufficient condition.

In the following we assume that a benzenoid is drawn so that some of its edges are vertical.

The concepts of horizontal cut segment and horizontal g-cut segment were introduced by the authors of Refs. 5 and 12, respectively. These concepts play an important role in the study of conditions for a benzenoid to be Kekuléan.[5,11,13] It is amazing that they are also very useful in the search for necessary and sufficient conditions for a Kekuléan benzenoid to be essentially disconnected.[8,12] Both of the above two concepts were defined for generalized benzenoids. When confined to benzenoids, defined in the usual way as in Ref. 3 or 6, they are as follows.

A horizontal straight line segment C with end points P_1, P_2 ($P_1 \neq P_2$) is called a horizontal cut segment of a benzenoid H if

(a) C is orthogonal to one of the three edge directions,

(b) each of P_1 and P_2 is the centre of an edge lying on the boundary of H,

(c) any point of C is either an interior or a boundary point of some hexagon of H,

(d) the graph obtained from H by deleting all edges intersected by C has exactly two components.

It is referred to Fig. 2 for an illustration.

A broken line segment $C=P_1P_2P_3$ (possibly, $P_2=P_3$) is called a horizontal g-cut segment of a benzenoid H if

(a) P_1P_2 is orthogonal to one of the three edge directions,

(b) each of P_1 and P_3 is the centre of an edge lying on the boundary of H, and if $P_2 \neq P_3$, P_2 is the centre of a hexagon of H,

(c) any point of C is either an interior or a boundary point of some hexagon of H,

(d) the graph obtained from H by deleting all edges intersected by C has exactly two components,

(e) if $P_2 \neq P_3$, the angle $P_1P_2P_3$ is $\pi/3$.

It is again referred to Fig. 2 (right-hand part).

In particular, if $P_2=P_3$, C becomes a horizontal cut segment. Therefore, we bear in mind that the term "horizontal g-cut segment" always includes horizontal cut segment as its special case.

For a horizontal g-cut segment $C=P_1P_2P_3$, let C_{12} and C_{23} denote the set of edges of H intersected by a straight line segment $C_{12}=P_1P_2$ and $C_{23}=P_2P_3$, respectively. Let $C=C_{12} \cup C_{23}$. C is called a horizontal g-cut. In particular, if $P_2=P_3$, $C=C_{12}$ is called a horizontal cut. Hence the term "horizontal g-cut" includes horizontal cut as its special case.

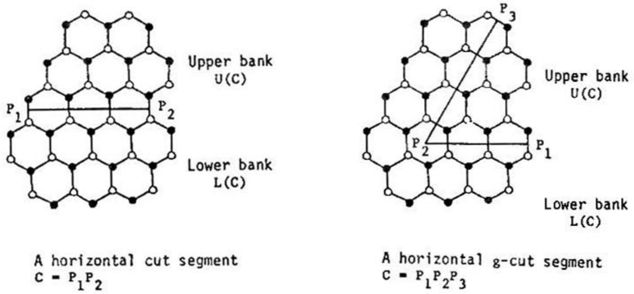


Fig. 2.

After deleting the edges in C, we get two components. They are called upper bank and lower bank (see Fig. 2).

BASIC FEATURE OF ESSENTIALLY DISCONNECTED BENZENOIDS

We notice that any essentially disconnected benzenoid must have some fixed single bonds, but may have no fixed double bonds (see Fig. 3). The figure shows the smallest essentially disconnected benzenoid, which has no fixed double bond.

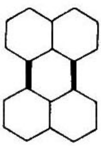


Fig. 3. The smallest essentially disconnected benzenoid (without fixed double bond). The fixed single bonds are drawn as heavy.

If an essentially disconnected benzenoid has some fixed double bonds, then the edges adjacent to these double bonds must be fixed single bonds. In other words, fixed double bonds are always accompanied by fixed single bonds. From this viewpoint we may say that fixed single bonds are the fundamental feature of essentially disconnected benzenoids. This is expressed in the following theorem.

Theorem 1. A Kekuléan benzenoid is essentially disconnected if and only if it has some fixed single bonds.

PREVIOUS RESULTS ABOUT THE CONDITION FOR A BENZENOID TO BE ESSENTIALLY DISCONNECTED

The authors of Ref. 12 investigated the problem when each hexagon of a benzenoid is resonant and found the following theorem as a by-product.

Theorem 2.[12] A Kekuléan benzenoid H has fixed bonds (single) if and only if there is at least one horizontal g-cut such that both of the two components of the graph obtained from H by deleting all the edges of the horizontal g-cut have Kekulé structures.

Since a benzenoid H is a bipartite graph, we can colour the vertices of H in two colours so that any two adjacent vertices are differently coloured. Without loss of generality, we may assume in the following that the peaks (i.e. the vertices lying above all their first neighbours) are coloured white, and the valleys (i.e. the vertices lying below all their first neighbours) are coloured black. It is not difficult to see that for any edge in a horizontal g-cut, the end-vertex lying in the upper bank is black, while that lying in the lower bank is white.

Let the number of edges in the set C_{12} be denoted by t, and the numbers of peaks and valleys of H lying in the upper bank by $n'_{\wedge}$ and $n'_{\vee}$, respectively. Denote $s=n'_{\wedge}-n'_{\vee}$. Cyvin and Gutman[8] proved the following theorems.

Theorem 3.[8] If for a Kekuléan benzenoid $s=t$ holds for at least one horizontal cut, the benzenoid is essentially disconnected.

Theorem 4.[8] If for a Kekuléan benzenoid $s=0$ holds for at least one horizontal cut, the benzenoid is essentially disconnected.

Theorem 2 describes a necessary and sufficient condition for a Kekuléan benzenoid to be essentially disconnected. Since it requires the knowledge of whether or not the two components (i.e. the upper bank and the lower bank) have Kekulé structures, this restricts the practical use of the theorem. The conditions in *Theorem 3* and *Theorem 4* are sufficient, but not necessary.[8]

A NECESSARY AND SUFFICIENT CONDITION

Before giving our main theorem we quote a useful theorem due to Hall.[14]

Theorem 5.[14] Let G be a bipartite graph with bipartition (X,Y). Then G has a matching that saturates every vertex in X if and only if $|N(S)|\geq|S|$ for all subsets $S\subseteq X$.

In the above theorem, N(S) is the neighbour set of S, i.e. the set of vertices which are adjacent to at least one vertex in S (see Fig. 4). The symbol $|S|$ denotes the number of vertices in a set S.

Now we are in the position to prove our main result.

Theorem 6. A Kekuléan benzenoid H has fixed single bonds if and only if $s=t$ holds for at least one horizontal g-cut.

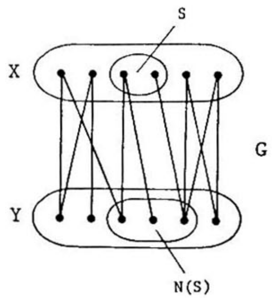


Fig. 4. A bipartite graph G with bipartition (X,Y), a subset $S \subset X$ and its neighbour set N(S).

Proof:

Sufficiency. Suppose that there is a horizontal g-cut C such that $s=t$ holds. We assert that all the edges in the horizontal g-cut C are fixed single bonds. Let W(U) and B(U) denote the sets of white and black vertices of the upper bank, respectively. It is not difficult to see that $|W(U)|-|B(U)|=n'_{\wedge}-n'_{\vee}-t=s-t=0$. This means $|W(U)|=|B(U)|$. Note that only the black vertices which are the end-vertices of the edges in C are adjacent to the white vertices in the lower bank; none of the white vertices in the upper bank is adjacent to a black vertex in the lower bank. Hence for any subset S of W(U), the neighbour set of S in H is just the neighbour set of S in the upper bank; hence for the number of vertices: $|N_U(S)|=|N_H(S)|$. Now by *Theorem 5* $|S|\leq|N_H(S)|=|N_U(S)|$. From $|S|\leq|N_U(S)|$, by the sufficiency of *Theorem 5*, for the upper bank U(H) there is a matching that saturates every vertex in W(U). It means that the upper bank U(H) has Kekulé structures. By a similar reasoning as above, the lower bank L(H) has Kekulé structures. Now by *Theorem 2*, H has fixed single bonds. Moreover, all the edges in the horizontal g-cut C are fixed single bonds.

Necessity: If H has fixed single bonds, by *Theorem 2* there is at least one horizontal g-cut such that both the upper and the lower banks have Kekulé structures. Thus $|W(U)|=|B(U)|$. Since $|W(U)|-|B(U)|=n'_{\wedge}-n'_{\vee}-t=s-t$, $s=t$ holds. ∎

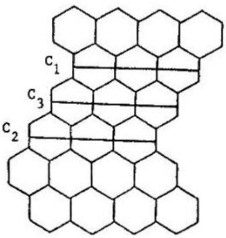
Combining *Theorem 1* and *Theorem 6*, the following statement is immediate.

Theorem 7. A Kekuléan benzenoid is essentially disconnected if and only if $s=t$ holds for at least one horizontal g-cut.

A SPECIAL KIND OF HORIZONTAL CUT

It is interesting that among all the examples given in Ref. 9 every essentially disconnected benzenoid has a horizontal cut such that $s=t$ holds and (at least) one of the two banks is a benzenoid, provided that the essentially disconnected benzenoid has some horizontal cut satisfying $s=t$. We call this special kind of horizontal cut a standard horizontal cut (see Fig. 5).

Fig. 5. An essentially disconnected benzenoid with two standard horizontal cuts (i.e. C_1 and C_2) corresponding to the horizontal cut segments c_1 and c_2, respectively) and a horizontal cut not being standard (i.e. C_3 corresponding to the horizontal cut segment c_3).



A standard horizontal cut is of great use in recognizing essentially disconnected benzenoids. It has a special location that is easy to find. It lies on the narrow part of the benzenoid (see Fig. 5). Moreover, the condition $s=t$ implies that the benzenoid obtained by deleting the standard horizontal cut has an equal number of peaks and valleys. This is easy to check. Therefore, it is easier to find a standard horizontal cut (if any) than an ordinary horizontal cut.

After inspecting all the essentially disconnected benzenoids with h (the number of hexagons) up to 8 (altogether 148 benzenoids),[9] one may have the impression that the existence of a standard horizontal cut is a general feature for essentially disconnected benzenoids having horizontal cuts which satisfy $s=t$. It is a fact, however, that an essentially disconnected benzenoid with a horizontal cut satisfying $s=t$ needs not to have a standard horizontal cut. Fig. 6 shows an example.

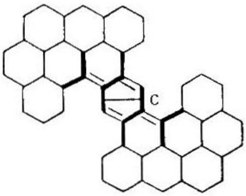


Fig. 6. An essentially disconnected benzenoid with a horizontal cut (C) satisfying $s=t$, but having no standard horizontal cut. (Heavy lines are fixed single bonds. Also the fixed double bonds are indicated.)

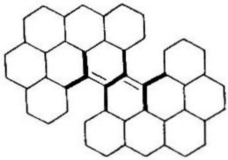


Fig. 7. An essentilaly disconnected benzenoid without a horizontal cut satisfying $s=t$.

SMALLEST ESSENTIALLY DISCONNECTED BENZENOIDS WITH CERTAIN CHARACTERISTICS

As pointed out in Ref. 9 an essentially disconnected benzenoid does not necessarily have a horizontal cut satisfying $s=t$. Fig. 7 shows an example given in the cited reference.[9]

It is natural to ask what the smallest essentially disconnected benzenoid without a horizontal cut satisfying $s=t$ is. In fact, the benzenoid depicted in Fig. 7 is just the smallest one. In the following we shall give a rigorous proof.

Theorem 8. There is a unique smallest (h=14) essentially disconnected benzenoid without a horizontal cut satisfying $s=t$, as is depicted in Fig. 7.

Proof:

Let H be a smallest essentially disconnected benzenoid without a horizontal cut satisfying $s=t$. Then H must have a horizontal g-cut C which is not a horizontal cut and satisfies $s=t$. It is not possible for the edges e_1 and e_2 to be on the boundary simultaneously (cf. Fig. 8a). We may assume that e_2 is on the boundary of H, while e_1 is not. This means that the hexagon s_1 belongs to H. Thus we have $n'_\wedge - n'_\vee = s = 1$. But $t=2$. Therefore, there must be some other hexagon on the upper bank of C. At least one hexagon, say s_2, belongs to H. If a hexagon s_3 does not belong to H, a horizontal cut would

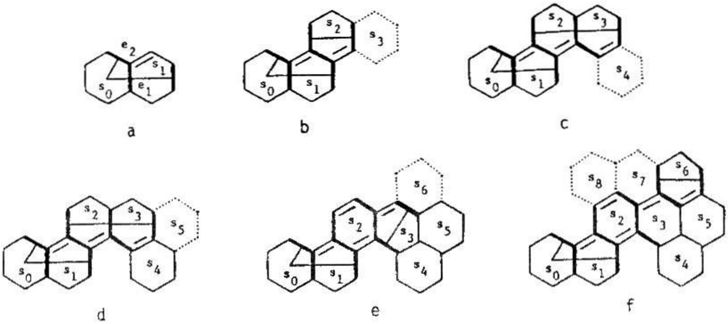
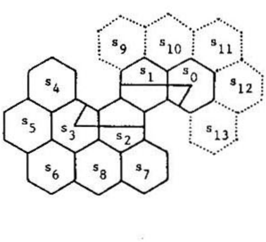


Fig. 8.

be found (Fig. 8b), a contradiction. Also the hexagon s_4 must belong to H; otherwise a horizontal cut would be found (Fig. 8c). Similarly the hexagon s_5 must belong to H (see Fig. 8d). Again, the hexagons s_6 and s_7 belong to H (see Figs. 8, e and f). Now, in order to fulfil the condition $s=t=2$, also at least the hexagon s_8 must belong to H. At this stage if we rotate the graph 180°, another horizontal g-cut is found (see Fig. 9). By arguing in a similar way as above, H must contain the hexagons s_9 to s_{13}. The proof is completed by realizing that the benzenoid which has emerged (Fig. 9), is just the one depicted in Fig. 7.

Another natural question is which benzenoid is the smallest one that has a horizontal cut satisfying $s=t$, but no standard horizontal cut satisfying $s=t$. The following theorem gives the answer.

Fig. 9.



Theorem 9. There is a unique smallest (h=15) essentially disconnected benzenoid which has a horizontal cut satisfying $s=t$, but no standard horizontal cut satisfying $s=t$. It is depicted in Fig. 6.

Proof:

Let H* be a smallest essentially disconnected benzenoid which has a horizontal cut satisfying $s=t$, but no standard horizontal cut satisfying $s=t$. Furthermore, let C be a horizontal cut of H* satisfying $s=t$. Since C is not standard, only one of the edges e_1 and e_2 belongs to H* (cf. Fig. 10a). We may assume that e_2 belongs to H*. By the minimality of H*, no other horizontal cut than C exists for H*. Hence a horizontal g-cut is found (Fig. 10b). Consider the lower bank of C*. By a similar reasoning as in the proof of *Theorem 8* the hexagons s_3 to s_7 must belong to H* (see Fig. 10c). Now rotate the graph 180°. Bear in mind that no other horizontal cut exists for H* by virtue of the minimality condition. By a similar reasoning as above we find that H* is just the benzenoid depicted in Fig. 6. ■

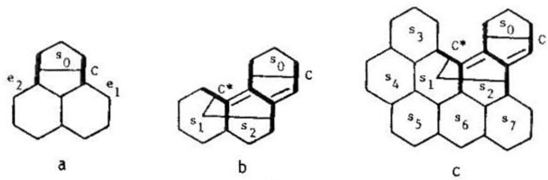


Fig. 10.

A SIMPLE CRITERION FOR ESSENTIALLY DISCONNECTED BENZENOIDS WITH $h \leq 14$

As mentioned in the preceding sections, a standard horizontal cut has several advantages in recognizing essentially disconnected benzenoids. By *Theorem 8*, any essentially disconnected benzenoid with $h \leq 14$ except the unique one depicted in Fig. 7 has a horizontal cut satisfying $s=t$. Furthermore, by *Theorem 9*, for any essentially disconnected benzenoid with $h<15$, if it has a horizontal cut satisfying $s=t$, then it must have a standard horizontal cut. This fact can be stated as the following theorem.

Theorem 10. A Kekuléan benzenoid with $h \leq 14$, which is not the one depicted in Fig. 7, is essentially disconnected if and only if it has a standard horizontal cut satisfying $s=t$.

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