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# ELEMENTARY EDGE–CUTS IN THE THEORY OF BENZENOID HYDROCARBONS

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**Abstract**

Some basic properties of elementary edge–cuts of benzenoid systems are established. If $r_i$ is the number of edges intersected by the $i$-th elementary edge–cut, $i = 1, 2, \ldots, \gamma$, then $[r_1, r_2, \ldots, r_\gamma]$ is the edge–cut sequence (ECS) of the respective benzenoid system. It is shown that a number of properties of a benzenoid system can be reconstructed from its ECS. We examine the conditions under which a sequence of integers is an ECS, and in the case of catacondensed benzenoids find a complete solution of this problem .

## Introduction

Edge–cuts were introduced into the theory of benzenoid systems by Horst Sachs [1], in connection with efforts to find necessary and sufficient conditions for the existence of Kekulé structures. These conditions were eventually discovered [2, 3] and, indeed, involve edge–cuts. Eventually, edge–cuts were used for recognizing and designing concealed non Kekuléan benzenoids [4, 5]. For review of research on non-Kekuléan benzenoid systems (in which edge–cuts play an outstanding role) see [6].

Edge–cuts have recently re-emerged in the theory of distance–related topological indices. It has been demonstrated that the Szeged ($Sz$) [7] and the Wiener ($W$) [8]

numbers of benzenoid hydrocarbons conform to the relations:

$$Sz = \sum_{i=1}^{\gamma} r_i \, n'(C_i) \, n''(C_i) \tag{1}$$

and

$$W = \sum_{i=1}^{\gamma} n'(C_i) \, n''(C_i) \tag{2}$$

in which $C_i$ stands for the $i$-th elementary edge-cut, dividing the benzenoid system into fragments with $n'(C_i)$ and $n''(C_i)$ vertices, and intersecting $r_i$ edges; the summations go over all elementary edge-cuts. The algebraic similarity between formulas (1) and (2) is remarkable. Eqs. (1) and (2) enable one to better understand the structure dependency of $Sz$ and $W$ [9, 10].

In spite of all these applications in the theory of benzenoid hydrocarbons, edge cuts were until now not subject of any systematic study. The aim of the present work is to contribute towards filling this gap.

In this paper we are concerned only with *elementary edge cuts*. These are defined as follows.

For our purposes benzenoid systems are viewed as geometric objects, obtained by arranging regular hexagons in the plane; for more details see [11], for an illustrative example see Fig. 1.

An elementary edge-cut is a straight line segment, drawn orthogonal to certain edges and passing through their centers. Each elementary edge-cut starts and ends at the perimeter, and must not have more than two points in common with the perimeter.

In Fig. 1 is depicted a benzenoid system and three of its elementary edge cuts. In diagram 1 the perimeter is indicated by heavy line. In diagram 2 the elementary edge-cuts are drawn strictly according to the above definition, with their ends indicated by heavy dots. In diagram 3 the same cuts are slightly extended; this is usually done in order to make their labeling easier.

Recall that the number of edges intersected by the elementary edge cut $C_i$ (including the two edges lying on the perimeter) is denoted by $r_i$. Thus, for the three cuts shown in Fig. 1, $r_1 = 4$, $r_2 = 2$ and $r_3 = 3$.

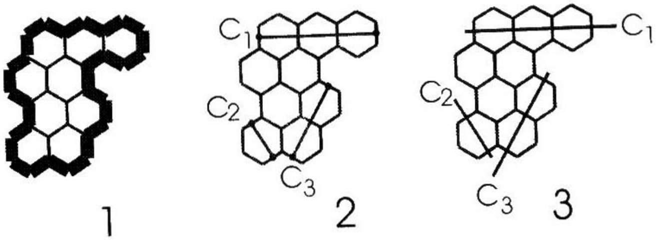


**Fig. 1**

Consider a benzenoid system $B$. Let $C_1, C_2, \ldots, C_\gamma$ be its elementary edge cuts. Suppose that they are labeled so that $r_1 \le r_2 \le \cdots \le r_\gamma$. Then the ordered $(\gamma)$-tuple $\mathbf{r}(B) = \mathbf{r} = [r_1, r_2, \ldots, r_\gamma]$ will be called the *edge cut-sequence* and abbreviated by ECS.

In Fig. 2 are shown the elementary edge-cuts of benzo[a]pyrene. There are nine such cuts, hence $\gamma = 9$. The respective ECS is [2,2,2,2,3,3,3,3,4].

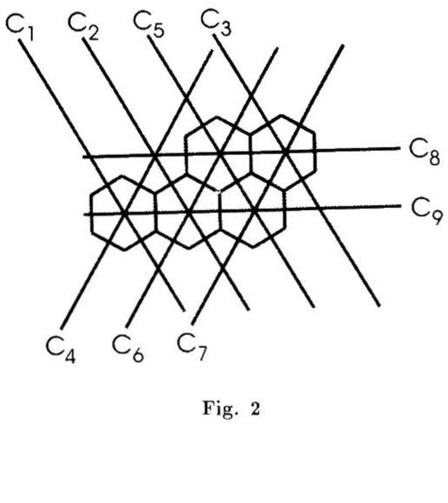


**Fig. 2**

In this paper we are interested in the following two questions:

**Problem 1.** Given $\mathbf{r}(B)$, what can be said about $B$ ?

**Problem 2.** Is a given sequence of integers an ECS of some benzenoid system?

## Some Elementary Results

We use the following notation [11]:

$n$ = number of vertices = number of carbon atoms,

$m$ = number of edges = number of carbon carbon bonds,

$h$ = number of hexagons,

$n_i$ = number of internal vertices,

$n_e$ = number of external vertices = size of perimeter,

$n_3$ = number of vertices of degree three,

$n_2$ = number of vertices of degree two = number of hydrogen-atoms.

**Proposition 1.** All the above listed quantities can be deduced from the ECS.

**Proof.** The above listed quantities can be calculated by means of the below given Eqs. (3)-(9).

First of all, the number of edges is evidently equal to the sum of the elements of the ECS:

$$m = \sum_{i=1}^{\gamma} r_i \ . \tag{3}$$

If an elementary edge–cut intersects $r_i$ edges, then it intersects $r_i - 1$ hexagons. Bearing in mind that each hexagon is intersected by three elementary edge–cuts, we conclude that

$$\sum_{i=1}^{\gamma}(r_i - 1) = 3h$$

i.e.,

$$h = \frac{1}{3}\left[\sum_{i=1}^{\gamma} r_i - \gamma\right] = \frac{m-\gamma}{3} \ . \tag{4}$$

¿From the well known Euler formula [11] $m = n + h - 1$, and using Eqs. (3) and (4) we now readily get

$$n = \frac{2m+\gamma}{3} + 1 \ . \tag{5}$$

Each elementary edge cut intersects exactly two edges that belong to the perimeter. Therefore $2\gamma$ is equal to the number of edges of the perimeter. Since the perimeter possesses equal number of vertices and edges, it follows that

$$n_e = 2\gamma \ . \tag{6}$$

Because $n_i = n - n_e$, by combining Eqs. (5) and (6) we arrive at

$$n_i = \frac{2m - 5\gamma}{3} + 1 \ . \tag{7}$$

The remaining two quantities from the above list are also readily calculated [11]:

$$n_3 = 2h - 2 = \frac{2m - 2\gamma}{3} - 2 \tag{8}$$

$$n_2 = n - n_3 = \gamma + 3 \tag{9}$$

by which the proof is completed. □

It is simple to see that for catacondensed benzenoids, for which $n_i = 0$ [11], the below statements are valid.

**Proposition 2.** If $B$ is a catacondensed benzenoid system with $h$ hexagons, then $B$ has $2h+1$ elementary edge-cuts, i.e., $\gamma = 2h + 1$. Furthermore,

$$n = n_e = 2\gamma$$

$$m = \frac{5\gamma - 3}{2}$$

$$n_3 = \gamma - 3$$

$$n_2 = \gamma + 3 \ .$$

**Proposition 3.** Consider a benzenoid system $B$ possessing $n$ vertices and $h$ hexagons. Let $r$ be an arbitrary element of $\mathbf{r}(B)$. Then $r$ is an integer, satisfying

$$2 \leq r \leq \frac{n+2}{4} \quad \text{and} \quad 2 \leq r \leq h + 1 \ .$$

**Proof.** Let $C$ be an elementary edge-cut of $B$, intersecting $r$ edges. Since $C$ intersects at least two edges (those belonging to the perimeter), it must be $r \geq 2$. Since $C$ intersects $r-1$ hexagons, it must be $r - 1 \leq h$ i.e., $r \leq h + 1$.

We now show that $B$ must possess at least $4r - 2$ vertices. Really, the $r-1$ hexagons intersected by $C$ form a subgraph of $B$ which is a linear polyacene. The linear polyacene with $h$ hexagons has $4h+2$ vertices [11]. Therefore the respective subgraph of $B$ has $4(r-1)+2 = 4r-2$ vertices, which, of course, is a lower bound for the vertex count of $B$. From $4r - 2 \leq n$ follows $r \leq (n+2)/4$. □

We mention in passing that the equality $r = (n+2)/4 = h+1$ is achieved if and only if $B$ itself is a linear polyacene.

## Edge–Cut Sequences as Partitions

Suppose that the benzenoid system considered has $h$ hexagons and $n_i$ internal vertices. Then, because of Eqs. (4) and (7), its edge-cut sequence has $\gamma = 2h + 1 - n_i$ elements, the sum of which is $m = 5h + 1 - n_i$. Bearing this in mind, we may consider an edge cut sequence as a partition of the number $m$ into $\gamma$ summands, each being an integer not smaller than two.

**Proposition 4.** Not all partitions of the number $5h + 1 - n_i$ into $2h + 1 - n_i$ summands, each being an integer not smaller than two, are edge cut sequences of benzenoid systems.

**Proof.** It is enough to construct a counterexample. Consider benzo[a]pyrene (see Fig. 2), for which $h = 5$ and $n_i = 2$ and $\mathbf{r} = [2,2,2,2,3,3,3,3,4]$. The latter is a partition of 24 into 9 summands. Another such partition is [2,2,2,2,2,2,2,2,8].

If [2,2,2,2,2,2,2,2,8] would be the ECS of a benzenoid system $B^*$, then by Proposition 1 $B^*$ would possess 5 hexagons. On the other hand, by Proposition 3, $B^*$ would possess at least 7 hexagons, a contradiction. □

The finding formulated as Proposition 4 is no surprise whatsoever. Much more unexpected is the following result.

**Proposition 5.** If $n_i = 0$ then all partitions of the number $5h + 1 - n_i = 5h + 1$ into $2h + 1 - n_i = 2h + 1$ summands, each being an integer not smaller than two, are edge–cut sequences of benzenoid systems.

**Proof.** We demonstrate the validity of a somewhat stronger statement, namely that for $h \geq 1$, every partition of $5h + 1$ into $2h + 1$ integers not smaller than 2 is an ECS of an unbranched catacondensed benzenoid system with $h$ hexagons.

Let $\mathbf{p} = [p_1, p_2, \ldots, p_{2h+1}]$ be a partition of $5h + 1$ into $2h + 1$ integers not smaller than two. We construct an unbranched catacondensed benzenoid system [11] $U$ with $h$ hexagons, such that $\mathbf{r}(U) = \mathbf{p}$.

If $h = 1$ then the unique partition of 6 into 3 integers not smaller than two is [2,2,2], being the ECS of benzene. Hence Proposition 5 holds for $h = 1$.

In what follows we assume that $h > 1$.

Denote by $\tau$ the number of elements of $\mathbf{p}$ which are equal to 2. The case $\mathbf{p} = [2,2,\ldots,2]$ is impossible because $2(2h+1) < 5h+1$. Therefore $\tau < 2h+1$ i.e., $\tau \leq 2h$.

Because $2\tau + 3(2h+1-t) \leq 5h+1$ it must be $\tau \geq h+2$. Therefore,

$$h + 2 \leq \tau \leq 2h \ . \tag{10}$$

Denote by $\mathbf{p}_2$ the sequence consisting of $\tau$ numbers which all are equal to 2. Let

$$\mathbf{p}^* = \mathbf{p} \setminus \mathbf{p}_2 \ . \tag{11}$$

Then $\mathbf{p}^*$ is a partition of the number $5h+1-2\tau$ into $2h+1-\tau$ integers not smaller than three.

An unbranched catacondensed benzenoid system consists of a certain number of angularly annelated (mode $A_2$) hexagons, a certain number of linearly annelated (mode $L_2$) hexagons and of two terminal (mode $L_1$) hexagons; for details see [11].

Denote by $h_A$ the number of angularly annelated hexagons of $U$.

For each hexagon of mode $A_2$ there is one elementary edge–cut with property $r_i = 2$. For other hexagons of $U$ there are two such cuts. Thus, $\mathbf{r}(U)$ will contain $\tau = \tau(U) = h_A + 2(h - h_A) = 2h - h_A$ elements equal to two.

For the remaining $h_A + 1$ elementary edge–cuts of $U$ we have $r_i \geq 3$. These correspond to the $h_A + 1$ linear segments of $U$ (i.e., maximal subgraphs that are linear polyacenes).

Choose $U$ so that $h_A = 2h - \tau(U)$. This is feasible because from (10) it follows that $0 \leq h_A \leq h - 2$. Then $\mathbf{r}$ possesses exactly $\tau(U)$ elements equal to two.

Denote by $u_1, u_2, \ldots, u_{h_A+1}$ the elements of $\mathbf{r}$ which are greater than two. Except that it must be

$$2\tau + \sum_{i=1}^{h_A+1} u_i = m(U) = 5h + 1$$

i.e.,

$$\sum_{i=1}^{2h+1-\tau} u_i = 5h + 1 - 2\tau \tag{12}$$

and, of course, $u_i \geq 3$, there is no restriction on the choice of the numbers $u_i$, $i = 1,2,\ldots,h_A+1$. In other words, any selection of integers not less than three, satisfying Eq. (12) may occur in some unbranched catacondensed benzenoid system.

This means that we always can find an unbranched catacondensed benzenoid system $U$, such that $[u_1, u_2, \ldots, u_{h_A+1}]$ is equal to any given partition of the number

$5h + 1 - 2\tau$ into $2h + 1 - \tau$ integers not smaller than three. In particular, we may always achieve that

$$[u_1, u_2, \ldots, u_{h_A+1}] \equiv \mathbf{p}^* \ . \tag{13}$$

We know that $\mathbf{r}(U)$ consists of $[u_1, u_2, \ldots, u_{h_A+1}]$ and additional $\tau$ elements which are equal to 2. In view of this, from Eqs. (11) and (13) one concludes that $\mathbf{p} \equiv \mathbf{r}(U)$.

By this Proposition 5 has been verified also for $h > 1$. □

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