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ESSENTIALLY DISCONNECTED BENZENOIDS: ENUMERATION AND CLASSIFICATION OF BENZENOID HYDROCARBONS - IX

J. BRUNVOLL, B.N. CYVIN, S.J. CYVIN and I. GUTMAN[a]

Division of Physical Chemistry, The University of Trondheim, N-7034 Trondheim-NTH, Norway. [a]On leave from *University of Kragujevac, Yugoslavia*

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Abstract: Essentially disconnected benzenoids are Kekuléan systems with fixed (single or double) bonds. In an essentially disconnected benzenoid the set of hexagons which contain fixed bonds defines the junction. The rest of the system consists of two or more effective units.

An exhaustive collection of 63 examples is given with a description of different structural features of the essentially disconnected benzenoids. The numbers of Kekulé structures (K) are given in all cases as the product of the Kekulé structure counts of the effective units.

Two theorems about essentially disconnected benzenoids are discussed.

The results of enumeration of essentially disconnected benzenoids for $h \leq 11$ are quoted. Here h is the number of hexagons. The classification into symmetry groups is quoted and supplemented.

All forms of the essentially disconnected benzenoids through h=8 (altogether 148 systems) are depicted and provided with K numbers.

DEFINITIONS AND INTRODUCTION

A benzenoid (defined in the usual way[1,2]) may be *Kekuléan* or *non-Kekuléan* depending on whether it has or has not Kekulé structures. *Essentially disconnected benzenoids*, the subject of the present work, are Kekuléan benzenoid systems with *fixed bonds*.

It may happen that an edge in a particular position is single or double in all Kekulé structures of a benzenoid. The fixed (single or double) bonds referred to above are just associated with such edges.

Although the existence of fixed bonds in benzenoids is long known,[3] they have not been exploited in the classification of the systems until recently. In the classical work on enumeration and classification of benzenoid systems by Balaban and Harary,[4] for instance, *perylene* (see Fig. 1) was counted together with the two other pericondensed[1,2,4] Kekuléan systems with h=5, viz. *benzo*[a]*pyrene* and *benzo*[e]*pyrene*. Here h is used (as usual) to designate the number of hexagons. These three h=5 benzenoids were referred to as "normal" (in a sense different from our definition; see below), in spite of the fact that *perylene* possesses two fixed single bonds. For h=6 the authors[4] placed *zethrene* (see Fig. 1) in a group of itself, not among the "normal" (Kekuléan pericondensed) benzenoids. This system has double (and single) fixed bonds. There are two additional systems with h=6 and fixed single bonds; they were again counted among the "normal" pericondensed benzenoids by Balaban and Harary.[4]

Fixed bonds were discussed (under the name "localized" bonds) also by Cyvin and Gutman.[5] These authors studied the K numbers of benzenoid systems with a single zigzag chain of hexagons. As a part of their work (among more general results) they produced an extrapolation of the *perylene-zethrene* systems in a different direction than the one of Fig. 1; see Fig. 2. Also all the members of the new homolog series (Fig. 2) have K=9.

The term "essentially disconnected benzenoid" was used for the first time by Cyvin et al.[6] during a systematic study of regular 5-tier strips. (See the cited work[6] for a precise definition of regular t-tier strips.) One class of essentially disconnected benzenoids is actually found also among the regular 3-tier strips;[7] it contains the *perylene-bisanthene* homologs as shown in Fig. 3. Two classes of essentially disconnected benzenoids are found among the regular 4-tier strips;[7] one of them is shown in Fig. 4.

The set of hexagons, in an essentially disconnected benzenoid, which possess fixed bonds, shall be referred to as the *junction*. The junction is usually a benzenoid or may be separated into two or more benzenoids. However, it may also be a coronoid.[8] The rest of the essentially disconnected benzenoid, i.e. when all edges with fixed bonds are deleted, consists of two or more fragments which shall be referred to as the *effective units*.

Let the effective units be denoted E_1, E_2, ... Then an essentially disconnected benzenoid in terms of its effective units may be written $E_1 \cdot E_2 \cdot \cdots\cdot$. This notation does not identify uniquely the form of the system, but its number of Kekulé structures is determined thereby. The K number of an essentially disconnected benzenoid is namely equal to the product of the Kekulé structure counts for the effective units (which behave independently with regard to the Kekulé structures);

$$K\{E_1 \cdot E_2 \cdot \cdots \cdot E_m\} = \prod_{i=1}^{m} K\{E_i\}$$

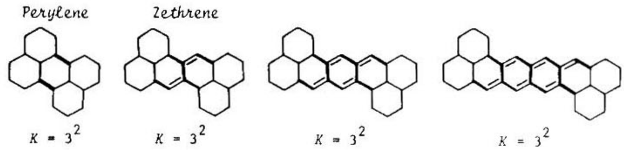


Fig. 1

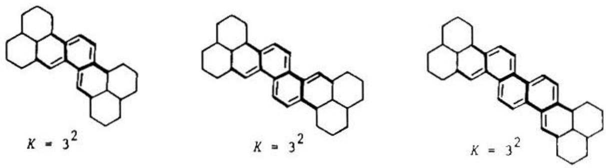


Fig. 2

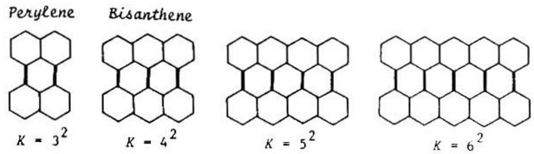


Fig. 3

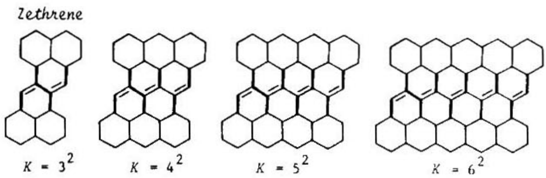


Fig. 4

The earliest studies of K numbers for classes of benzenoids[9,10] contain some classes of essentially disconnected benzenoids. Gordon and Davison[9] have given the formula $K = (n+1)^2$ for the class of Fig. 3. Here n is given by $L(n) \cdot L(n)$, where the effective units are specified as single linear chains (*polyacenes*) of n hexagons. Yen[10] gave a generalization of the mentioned K formula, considering a class of benzenoids later referred to as prolate rectangles;[11] cf. Fig. 5. In none of the two early works[9,10] there is any explicit mentioning of fixed bonds. The development of Yen's formula in particular is said to be "based on combinatorial mathematics",[10] without any details of the derivation. When the prolate rectangle (Fig. 5) is characterized by

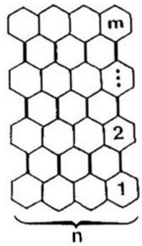
L(n)·L(n)· ····, we obtain immediately, since $K\{L(n)\} = n+1$,[9]

$$K\{L(n)\cdot L(n)\cdot \cdots\cdot (m \text{ times})\} = (n+1)^m$$

which is the formula of Yen.[10]

The *neo* classification[12,13] is appropriate in the studies of Kekulé structure counts of benzenoid systems. All benzenoids are covered by the categories *normal* (n), essentially disconnected (e) and non-Kekuléan (o) systems.

Fig. 5



Here a normal benzenoid is defined strictly as a Kekuléan benzenoid which is not essentially disconnected (i.e. does not possess any fixed bond). The *neo* classification has been employed in enumerations of benzenoids with increasing values of h (numbers of hexagons).[13-16] Enumerations of benzenoids with hexagonal[17,18] and trigonal[19] symmetries have been executed specifically. Also in these enumerations the *neo* classification plays an important role.

All essentially disconnected benzenoids are pericondensed systems. The effective units are normal (catacondensed[1,2,4] or pericondensed). Cyvin and Gutman[20] tried to give a further characterization of essentially disconnected benzenoids in terms of a segmentation procedure. They found some useful sufficient conditions for a benzenoid to be essentially disconnected, but no necessary and sufficient condition.

In Figs. 1-5 the fixed single and double bonds are drawn as heavy and double lines, respectively.

EXAMPLES OF DISCONNECTED BENZENOID SYSTEMS (GENERALIZED BENZENOIDS)

Biphenyl (see Fig. 6) is the smallest system with a fixed (single) bond. The class of Fig. 3 degenerates to *biphenyl* for n=1. More generally, the prolate rectangles (Fig. 5) degenerate to *polyphenylenes*, L(1)·L(1)· ···· with $K = 2^m$, as already was pointed out by Yen.[10] The last (right-hand side) example of Fig. 6 is the degenerated case of n=1 for the class of Fig. 4.

The systems of Fig. 6 may be described as benzenoids (corresponding to effective units) joined by chains of acyclic edges (with fixed bonds, the

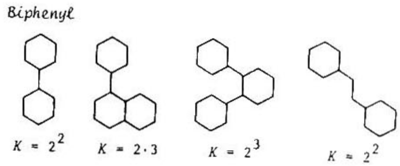


Fig. 6

degenerated junctions) and termed *disconnected benzenoid systems*. The whole system of a number of disconnected benzenoids in the described way is not a benzenoid according to the strict definition of the concept. However, it falls under the definition of a generalized benzenoid due to Sachs[21] (actually termed "generalized hexagonal system" therein).

EXAMPLES OF ESSENTIALLY DISCONNECTED BENZENOIDS

This section is supposed to be a contribution to the "anatomy" of "hexagonal animals". The concept "hexagonal animal"[22,23] is synonymous with "benzenoid" among a plethora of other designations.[1,2] We shall show a diversity of examples of essentially disconnected hexagonal animals and point out some of their features.

The systems with K=9 are not restricted to the classes of Fig. 1 and Fig. 2. As pointed out by Cyvin and Gutman[5] the single chain constituting the junction may be varied arbitrarily. Two examples are depicted in Fig. 7. Also the effective units may be substituted by an infinite number of normal benzenoids, catacondensed or pericondensed; see the examples of Fig. 8.

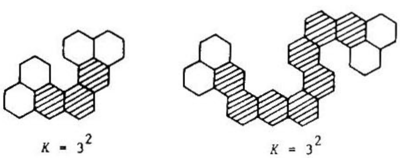


Fig. 7

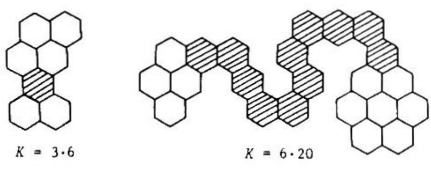
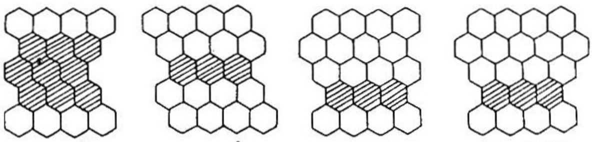


Fig. 8

It was mentioned above that there are two classes of essentially disconnected benzenoids among regular 4-tier strips. One of them is specified in Fig. 4, while the first member (n=2) of the other is found in Fig. 8 (left). Several varieties occur among the ten classes of essentially disconnected benzenoids among regular 5-tier strips.[6] Four examples from different classes are shown in Fig. 9.



$K = 5^2$ $K = 15^2$ $K = 5 \cdot 55$ $K = 5 \cdot 105$ Fig. 9

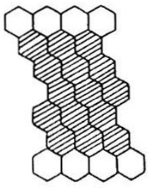


Fig. 10 $K = 5^2$

In the extreme left system of Fig. 9 the junction is a multiple chain.[6] It has been demonstrated[5] that also this type of junction may be varied infinitely like the single chain, without affecting the K number, although the multiple chain is not so flexible. Fig. 10 shows an example to be compared with the extreme left system of Fig. 9.

Many other forms of the junction of an essentially disconnected benzenoid are possible. Cyvin and Gutman[5] have indicated some principles for construction of various junctions. They gave two examples similar to those of Fig. 11. Some additional forms are depicted in Fig. 12.

In all the above examples of essentially disconnected benzenoids except the prolate rectangle for $m > 2$ (viz. in Figs. 1-4 and Figs. 7-12) each system has exactly two effective units. There are several examples with more than two effective units in the following. At the present stage we wish only to mention, in connection with the prolate rectangles (Fig. 5), that any of the fixed (single) bonds may be deleted without affecting the K number, which is $(n+1)^m$ (see above). Fig. 13 (middle drawing) shows an essentially disconnected benzenoid produced in this way from the left-hand system of the same figure. In Fig. 13 the right-hand system exemplifies that the rule also applies when generalized benzenoids are obtained in the process. This rule of deleting fixed single bonds without affecting the K number is quite general.

In Figs. 7-13 the junctions of the depicted essentially disconnected benzenoids are hatched. The same identification is also to be used in several figures in the following.

In absolutely all of the above examples of essentially disconnected benzenoids (Figs. 1-5, Figs. 7-12 and the two left-hand systems of Fig. 13) the effective units are coupled to the junction through a single or multiple condensation. We say that two benzenoids are (simply) condensed when they share exactly two incident edges. In the present context, when an effective unit is simply condensed with the junction, a hexagon of the junction is inserted into a fissure (formed by two incident edges belonging to different hexagons) of the effective unit. Here the internal vertex belonging to both the effective unit and the junction is of particular interest. Cyvin and Gutman[5] considered in detail the cases where two *naphthalene* units are condensed to a single chain. Fig. 14 exemplifies how such systems may be realized in four ways for a given chain (with at least 3 hexagons). In these special cases the vertices of interest are the only two internal vertices for the

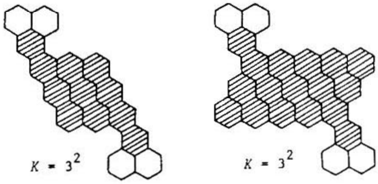


Fig. 11

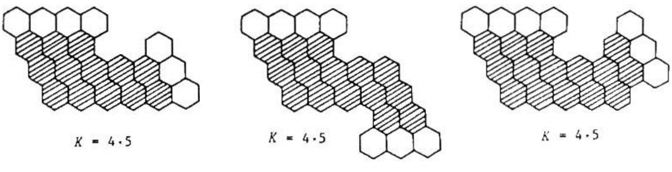


Fig. 12

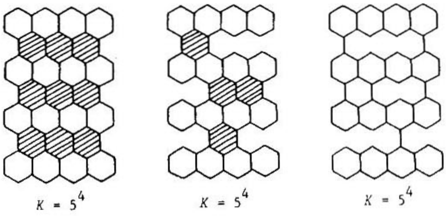


Fig. 13

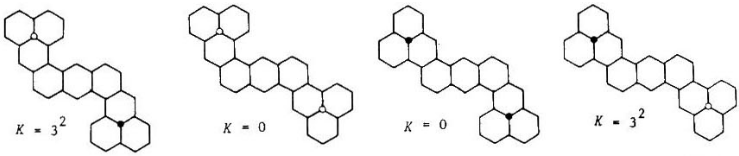


Fig. 14

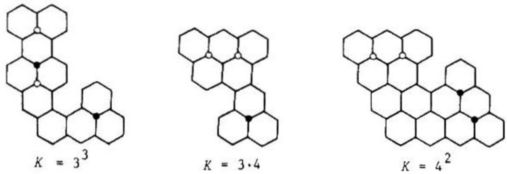


Fig. 15

whole system. The authors[5] stated the rule that a system of the considered type is essentially disconnected (with K=9) when the two internal vertices are of different colors and non-Kekuléan if they are of the same color. In the latter case the system is obvious non-Kekuléan.[20] Similar rules are valid for multiple condensation (when two or more fissures of an effective unit are involved) and systems of more than two effective units condensed to the junction; cf. Fig. 15, where all the depicted systems are essentially disconnected benzenoids.

This "anatomic" study of essentially disconnected hexagonal animals would not be complete without pointing out that an effective unit may be connected with the junction in other ways than the (single or multiple) condensation.

Suppose that an essentially disconnected benzenoid has been established, and the junction possesses a free edge (i.e. an edge between two vertices of second degree). Assume that a hexagon is fused to this edge. If the edge is associated with a (fixed) single bond, then the fused hexagon will only add to the junction. If, however, the edge is associated with a (fixed) double bond in the original system, then the fusion will annihilate the fixed nature of this bond, and the new hexagon will form an additional effective unit. (This hexagon acquires a mode which is designated L_1.) In Fig. 16 these features are illustrated for the simplest cases. One hexagon is added to the first system of Fig. 2 (see the left-hand drawing of Fig. 16) and to the first system of Fig. 7 (see the right-hand drawing of Fig. 16).

Fig. 17 shows four essentially disconnected benzenoids with three effective units each. The number of hexagons (h) is indicated for the two sys-

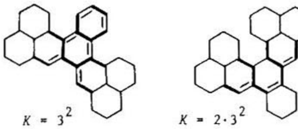


Fig. 16

tems which are supposed to be the smallest existing of this kind. Only in the two last (right-hand) systems a fusion to the junction is present. The next-to-last system is identical with the last one of Fig. 16. Similarly to Fig. 17 some systems with four effective units each are shown in Fig. 18. Notice that the presumably smallest (h=10) systems of this kind have less hexagons than the prolate rectangle with four *naphthalene* units. Also the examples of Fig. 19 are illuminating. The two last (right-hand) systems therein are the smallest essentially disconnected benzenoids with five and

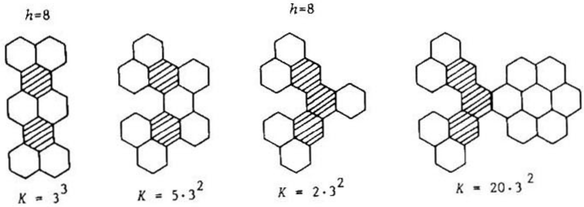


Fig. 17

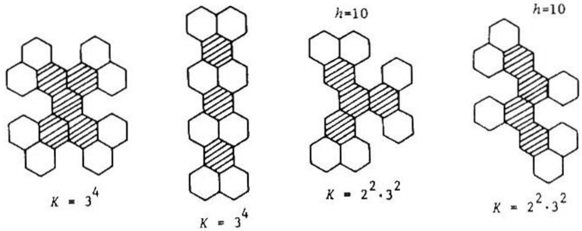


Fig. 18

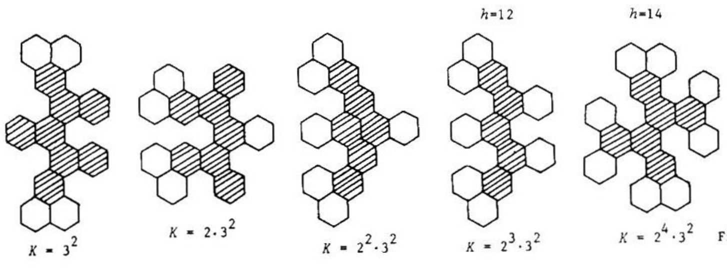


Fig. 19

six effective units, respectively, which we have been able to find by trial and error.

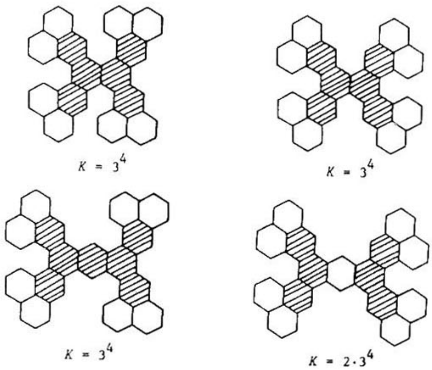
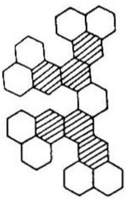


Fig. 20

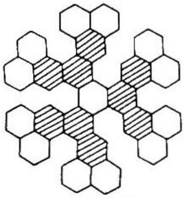
Fig. 20 shows two essentially disconnected benzenoids with h=14 (top row) and two with h=15 (bottom row). The bottom-right system displays a new feature: a two-sided annelation (or fusion) of parts of the junction to one and the same hexagon (*benzene*), which constitutes one of the effective units. This hexagon experiences a linear annelation. Fig. 21 shows that also an angular annelation and even a three-sided annelation is possible. (The pertinent hexagon is said to have the modes L_2, A_2 and A_3, respectively, in the three cases.)

This brings us to the description of cases where the connection between the junction and an effective unit is still more intricate. Fig. 22 shows three diverse examples. The first of them illustrates an interesting principle. The system may be produced by fusing a benzenoid (*coronene*) to the free edge associated with a fixed single bond of the junction of the first system of Fig. 2. The corresponding fusion of one hexagon (Fig. 16) added this hexagon to the junction. In the present case (Fig. 22) the junction is extended again, but not by the whole added benzenoid. In this way the new junction is imbedded into a bay (formed by three incident edges) of the new effective unit (*benzo*[ghi]*perylene*). The next (middle) drawing illustrates the opposite instance, where an effective unit (*pyrene*) fills up some bays of two parts of the junction. In the right-hand picture (Fig. 22) the junction fills up coves (formed by four incident edges) in addition to fissures of the effective units.

Finally in this section we show some cases where one of the effective units is almost or completely surrounded by the junction (Fig. 23). In the latter case, if the pertinent effective unit is larger than one hexagon, the junction is a coronoid. This feature was discovered for the first time during the enumeration of benzenoids with hexagonal symmetry,[17,18] but only with one hexagon (*benzene*) as the surrounded effective unit (cf. the left drawing of Fig. 24). As the last example (Fig. 24) we have depicted a larger essentially disconnected benzenoid with hexagonal symmetry, where the junction actually is a coronoid.



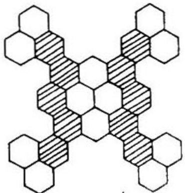
$K = 2\cdot 3^4$



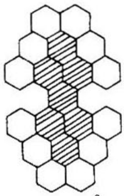
$K = 2\cdot 3^6$

Fig. 21

$K = 14\cdot 3^2$

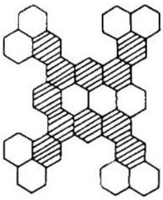


$K = 6\cdot 3^4$

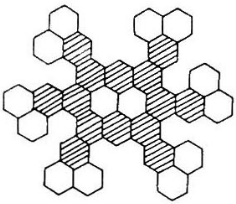


$K = 15^2$

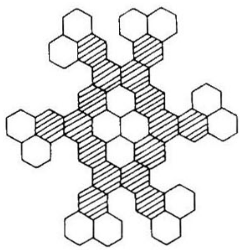
Fig. 22



$K = 4\cdot 3^4$

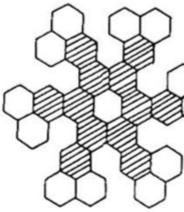


$K = 3^7$

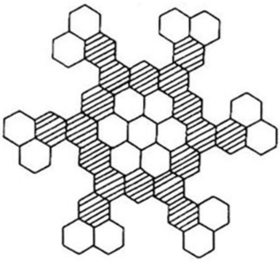


$K = 6\cdot 3^6$

Fig. 23



$K = 2\cdot 3^6$



$K = 20\cdot 3^6$

Fig. 24

TWO THEOREMS ABOUT ESSENTIALLY DISCONNECTED BENZENOIDS

Cyvin and Gutman[20] have proved two theorems about essentially disconnected benzenoids on the basis of a segmentation procedure. They are quoted in the following after some necessary preparations (for supplementary definitions, see, e.g. the cited reference[20]).

Assume that a benzenoid system is drawn (as usual) so that some of the edges are vertical. An (elementary) *edge-cut* is a horizontal line through a set of vertical edges, the end edges belonging to the perimeter.[24] The cut edges are referred to as *tracks*. Their number is identified by the symbol t. The horizontal line divides the system into the upper and lower *segment*. Notice that the segments are not actually separated, in contrast to other approaches to the problem.[21,24] Let the numbers of peaks and valleys of the upper segment be denoted by $n_\wedge'$ and $n_\vee'$, respectively. Correspondingly $n_\wedge''$ and $n_\vee''$ for the lower segment.

Kekuléan (and concealed non-Kekuléan) benzenoids possess equal number of peaks and valleys, i.e. $n_\wedge' + n_\wedge'' = n_\vee' + n_\vee''$. Therefore,

$$n_\wedge' - n_\vee' = n_\vee'' - n_\wedge''$$

The above differences will be denoted by s and may be termed the partial difference of the numbers of valleys and peaks for that particular segmentation.

Two theorems:

(1) If for a Kekuléan benzenoid

$s=t$ in at least one segmentation (a)

the benzenoid is essentially disconnected.

(2) If for a Kekuléan benzenoid
s=0 in at least one segmentation (b)
the benzenoid is essentially disconnected.

The theorems represent two sufficient conditions, which characterize an essentially disconnected benzenoid.

In the case of (1) all the tracks are associated with single bonds.[20] In the case of (2) all the tracks are associated with double bonds.[25]

In Fig. 25 we show two examples (cf. Fig. 7 and Fig. 18) where both conditions (a) and (b) are realized. The peaks and valleys are colored white and black, respectively. Notice that it is expedient, in order to gain most information, to cut the edges at the thinnest part.

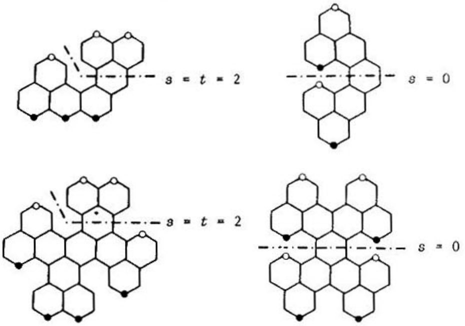


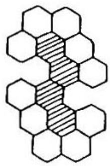
Fig. 25

Cyvin and Gutman[20] left it as an open question whether the condition (a) is a necessary condition for an essentially disconnected benzenoid, i.e. if it always is realized in at least one segmentation in one of the three different orientations. On the other hand the authors[20] demonstrated easily that the condition (b) is not necessary; counterexample: *perylene*.

In the whole collection of 62 examples of the preceding section there is only one counterexample to the necessity of condition (a). In the last (right-hand) system of Fig. 22 $s=t$ (a) is never realized, but so is s=0 (b).

Hence the question arises naturally whether either (a) $s=t$ or (b) s=0 (or both) is necessarily realized for any essentially disconnected benzenoid. The material of the preceding section does not present any counterexample, but one has been found as is displayed in Fig. 26. For this benzenoid none of the two conditions can possibly be realized inasmuch as it is impossible to execute an (elementary) edge-cut through fixed bonds only.

Hence we conclude that the requirement (a) *or* (b) *is a sufficient, but not a necessary* and *sufficient condition for a benzenoid system to be essentially disconnected.* Thus the finding of necessary and sufficient structural requirements for essentially disconnected benzenoids, or, what is the same, the finding of an easy procedure for recognizing whether a given benzenoid is essentially disconnected or not, remains an open problem of the topological theory of benzenoid systems.



$K = 11^2$ Fig. 26

ENUMERATION OF ESSENTIALLY DISCONNECTED BENZENOIDS

Table 1 shows the results of enumeration of essentially disconnected benzenoid systems. The distributions into symmetry groups are indicated. The previous data from literature (according to the footnotes of Table 1) were supplemented by new computer runs. The data are complete for $h \leq 11$. Specific runs for the different symmetries except C_s were executed in order to extend some of the data to higher h values. Additional data (not quoted in Table 1) are available for the C_{6h} symmetry group up to h=43,[17] and for D_{6h} up to h=55.[18]

FORMS OF ESSENTIALLY DISCONNECTED BENZENOIDS

A systematic survey of all essentially disconnected benzenoids with $5 \leq h \leq 8$ is given in Fig. 27 in terms of black silhouettes on the background of the hexagonal lattice. They are ordered according to increasing K numbers.

CONCLUSION

The present work is supposed to give a better insight into the nature of the peculiar systems referred to as essentially disconnected benzenoids.

The extensive collection of examples, showing the diversity of forms, could not have been produced without the computer-aided enumerations. The specific enumerations for different symmetries proved to be especially use-

Table 1. Numbers of essentially disconnected benzenoids, classified according to symmetry.

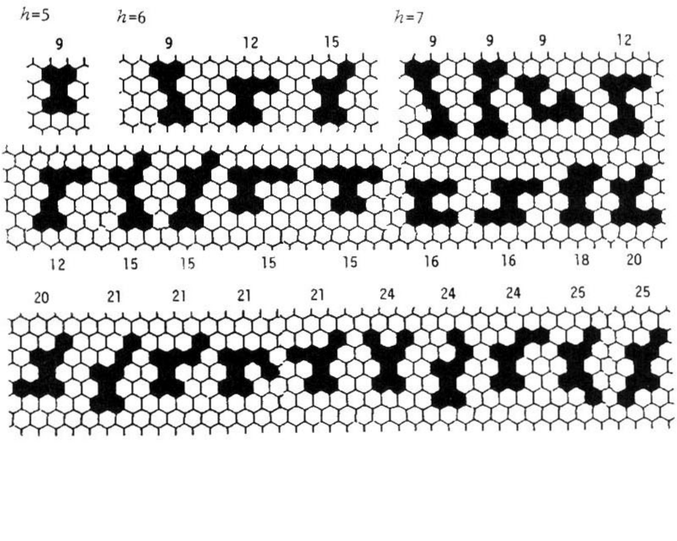
h	D_{6h}	C_{6h}	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}	C_s	Total
5	0	0	0	0	1[a]	0	0	0	1[b]
6	0	0	0	0	0	1[a]	0	2[a]	3[b]
7	0	0	0	0	0	3[a]	6[a]	14[a]	23[b]
8	0	0	0	0	2[a]	7[a]	2[a]	110[a]	121[b]
9	0	0	0	0	2[a]	16[a]	29[a]	645[a]	692[b]
10	0	0	0	0	1[a]	53[a]	31[a]	3647[a]	3732[c]
11	0	0	0	0	2	87	166	19705	19960[c]
12	0	0	0	0	5				
13	0	0	0	0	7				
14	0	0	0	0	7				
15	0	0	0	0	9				
16	0	0	1[d]	2[d]	19				
17	0	0	0	0	27				
18	0	0	0	0	34				
19	0	0	0	23[d]	39				
20	0	0	0	0	84				
21	0	0							
22	0	0							
23	0	0							
24	0	0							
25	1[a]	1[a]							

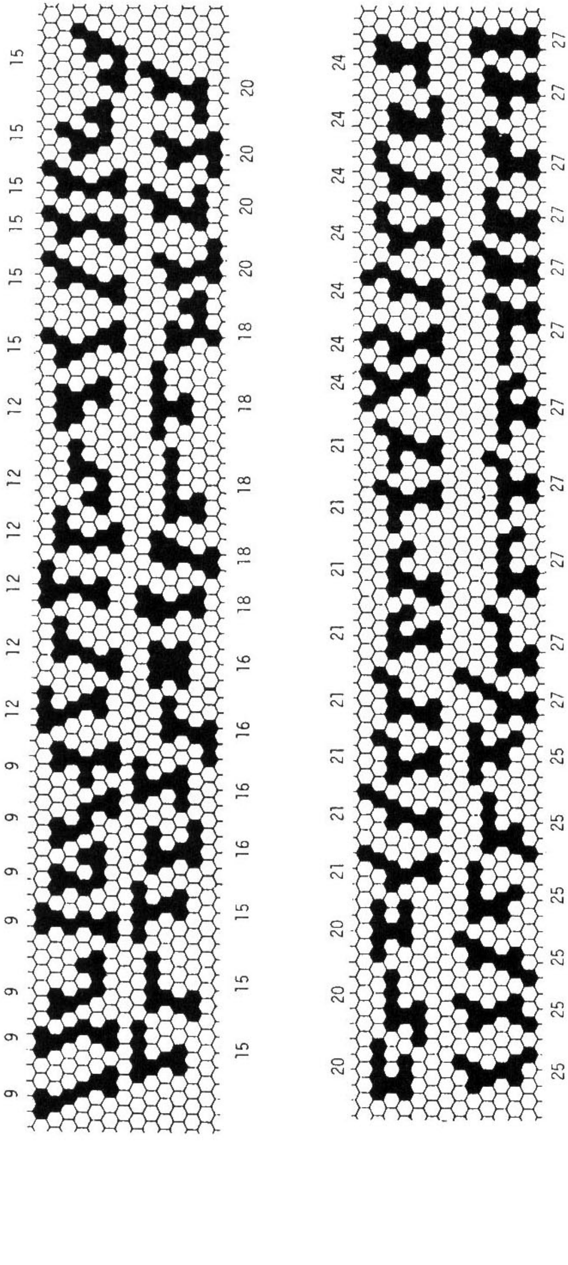
[a]Ref. [17]

[b]Ref. [14]

[c]Ref. [16]

[d]Ref. [19]





$h=8$

(h=8 cont.)

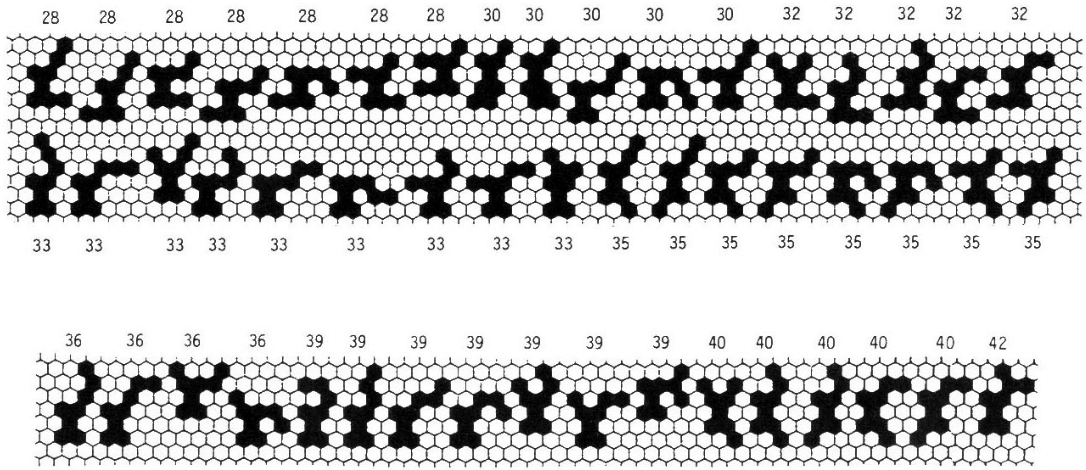


Fig. 27 (see also the two preceding pages). All essentially disconnected benzenoids with h (the number of hexagons) up to 8. K numbers (Kekulé structure counts) are given.

ful inasmuch as they could be carried through substantially larger h values than the enumerations of benzenoids in total, and they revealed several new features.

A simple algorithm for recognizing any essentially disconnected system, involving necessary and sufficient conditions, is not yet known. The present material may be useful for creating new ideas, search for counter-examples, etc.

Essentially disconnected benzenoids have proved to be very useful in certain K enumeration techniques[26,27] based on the fragmentation method of Randić.[28]

In a recently published book by Cyvin and Gutman[27] there is a chapter on essentially disconnected (and non-Kekuléan) benzenoid systems. The present paper is complementary to that chapter and contains many more details.

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