Concealed Non-Kekuléan Benzenoids

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A concealed non-Kekuléan benzenoid (CNB) is a benzenoid with the same number of starred and unstarred (black and white) vertices but no Kekulé structure. The search for CNBs was pursued to h (number of hexagons) = 16 by computer programming. For h = 14, the previously controversial number of 9804 systems was confirmed by a construction method without use of computers. In the Appendix, the previously deduced numbers for concealed non-Kekuléan helicenes with h = 11, 12, and 13 by the construction method are verified by new computer enumerations.

INTRODUCTION

The existence or nonexistence of Kekulé structures[1] in benzenoids[2] is an important property from the chemical point of view. At the same time it is a basis for distinguishing between two main classes of benzenoids: Kekuléan and non-Kekuléan. The non-Kekuléan benzenoids are further subdivided into the obvious and concealed non-Kekuléans.[1,2] Concealed non-Kekuléan benzenoids, the topic of the present work, are characterized by $K = 0$ and $\Delta = 0$, where K is the Kekulé structure count and Δ is the color excess.[2] In other words, a concealed non-Kekuléan (benzenoid) has no Kekulé structure but the same number of starred and unstarred (or black and white) vertices and therefore also the same number of peaks and valleys. Helicenes (polyhexes with overlapping edges) are not included among benzenoids according to the definitions adopted here. Concealed non-Kekuléan helicenes, mentioned in the Appendix, are defined in the same way as the concealed non-Kekuléan benzenoids.

Already in 1972 Clar[3] furnished a precise characterization of what we now call a concealed non-Kekuléan benzenoid when he described the $C_{38}H_{18}$ hydrocarbon which corresponds to one of the systems depicted in Figure 1 (at the extreme upper right). Since then the search for concealed non-Kekuléans has been going on. Gutman[4] and Balaban[5,6] were among those who contributed to this search. But it took 14 years before Hosoya[7] (in 1986) and other authors[8] independently depicted eight nonisomorphic concealed non-Kekuléan benzenoids with eleven hexagons each (h = 11). Shortly thereafter Brunvoll et al.[9] demonstrated by running a computer program that these eight systems are exactly the smallest (h = 11) nonisomorphic concealed non-Kekuléans. Furthermore, Zhang and Guo[10] supplied a graph-theoretical proof to the same effect. We shall not repeat the long story of the search for concealed non-Kekuléan benzenoids.[11,12] A most detailed account is found in a recent review.[13] Herein it is referred to a concealed non-Kekuléan given by Dias,[14] which is the first $C_{44}H_{22}$ system on Figure 1.

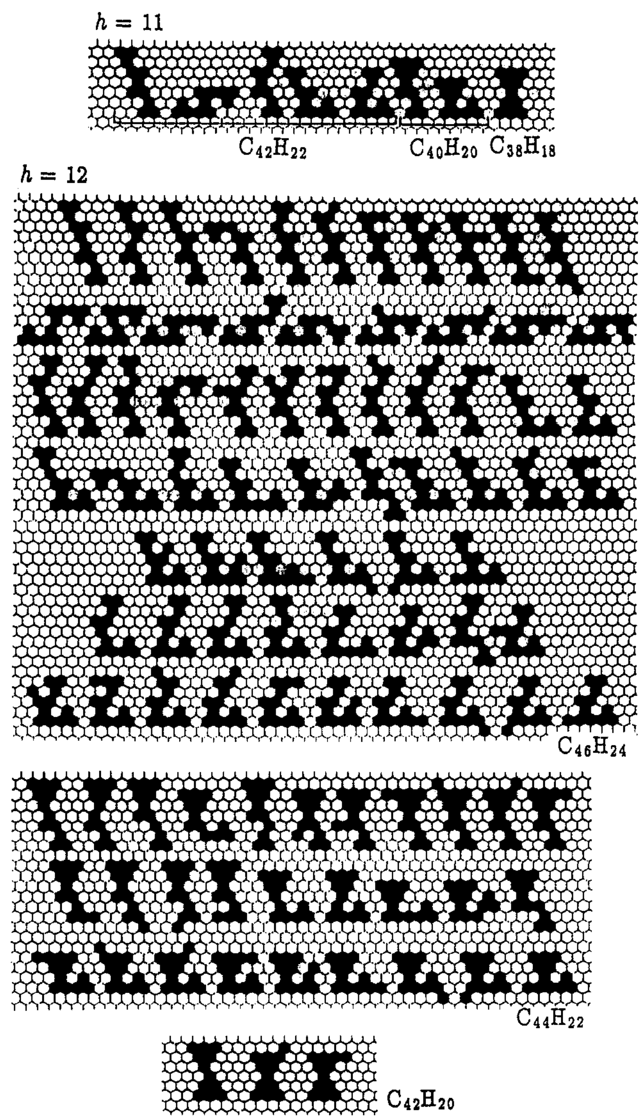

Figure 1. The forms of the concealed non-Kekuléan benzenoids with h = 11 and 12.

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Table 1. Numbers of Concealed Non-Kekuléan Benzenoids Classified According to Symmetry

h	D_{2h}	C_{2h}	C_{2v}	C_s	total
11	1[a]	2[b]	1[b]	4[b]	8[c]
12	0	5[b]	0	93[b]	98[d]
13	0	23[e]	23[e]	1051[e]	1097[f,g]
14	1[a]	58[e]	11[e]	9734[e]	9804[e]
15	3[a]	177[e]	185[e]	78126	78491
16	3[a]	502[e]	145[e]	575838	576488

[a] Gutman and Cyvin (1988).[24] [b] Gutman and Cyvin (1989).[2] [c] Brunvoll et al. (1987).[9] [d] He et al. (1988).[25] [e] Cyvin et al. (1992).[13] [f] Guo and Zhang (1989).[26] [g] Jiang and Chen (1989).[15]

Table 2. Chemical Formulas (C_nH_s) for Concealed Non-Kekuléan Benzenoids

	n_i						
h	4	6	8	10	12	14	16
11	$C_{42}H_{22}$	$C_{40}H_{20}$	$C_{38}H_{18}$				
12	$C_{46}H_{24}$	$C_{44}H_{22}$	$C_{42}H_{20}$				
13	$C_{50}H_{26}$	$C_{48}H_{24}$	$C_{46}H_{22}$	$C_{44}H_{20}$			
14	$C_{54}H_{28}$	$C_{52}H_{26}$	$C_{50}H_{24}$	$C_{48}H_{22}$	$C_{46}H_{20}$		
15	$C_{58}H_{30}$	$C_{56}H_{28}$	$C_{54}H_{26}$	$C_{52}H_{24}$	$C_{50}H_{22}$		
16	$C_{62}H_{32}$	$C_{60}H_{30}$	$C_{58}H_{28}$	$C_{56}H_{26}$	$C_{54}H_{24}$	$C_{52}H_{22}$	$C_{50}H_{20}$

In the cited review,[13] a controversy is reported: for h = 14 Jiang and Chen[15] found 9781 concealed non-Kekuléan benzenoids by a paper-and-pencil method (without rigorous proofs), while a computer enumeration[13] came out with the number 9804. In the present work, the latter number (viz. 9804) is confirmed by another paper-and-pencil method involving constructions and supported by rigorous proofs. Additional computer enumerations for the non-Kekuléans were also executed in the present work, whereby the previously known numbers[13] were reproduced and supplemented considerably.

COMPUTERIZED ENUMERATIONS

Principles. A computer program for generation and enumeration of benzenoids was devised on the basis of the DAST (dualist angle-restricted spanning tree) code,[16,17] which has proved to be very efficient.[18] All the 74 207 910 benzenoids with h = 15 and 359 863 778 benzenoids with h = 16 were generated in consistency with the previously reported numbers,[16-18] but the systems were subjected to a detailed classification for the first time. The determination of symmetry groups was included.[19] In particular, the concealed non-Kekuléans were recognized among other benzenoid classes. A count of the internal vertices made it feasible to determine the numbers of C_nH_s isomers.[20-23]

Results. The numbers of nonisomorphic concealed non-Kekuléan benzenoids with $h \leq 16$ are given in Table 1. The distribution into symmetry groups is included therein. Figure 1 shows the forms of the systems under consideration with h = 11 and 12. For each h, several C_nH_s isomers are represented among the concealed non-Kekuléans, as is exemplified in Figure 1. In Table 2, all the formulas which are possible for the concealed non-Kekuléan benzenoids with $h \leq 16$ are listed. The corresponding numbers of isomers are given in Table 3.

CONSTRUCTION METHOD

Introductory Remarks. The construction method for concealed non-Kekuléan benzenoids which was developed

Table 3. Numbers of C_nH_s Isomers of Concealed Non-Kekuléan Benzenoids

	n_i						
h	4	6	8	10	12	14	16
11	5[a]	2[a]	1[a]				
12	66[b]	29[b]	3[b]				
13	752[c]	299[c]	43[c]	3[c]			
14	6585[c]	2696[c]	478[c]	44[c]	1[c]		
15	50727	22288	4867	570	39		
16	353086	172406	44100	6337	539	19	1[c]

[a] Hosoya (1986).[7] [b] He et al. (1988).[25] [c] Brunvoll et al. (1992).[23]

by Zhang and Guo[10] is based on the necessary and sufficient conditions for a benzenoid to have Kekulé structures.[27,28] No computer programming is involved, and yet the construction method can be used to deduce quite large numbers of concealed non-Kekuléans. After proving that there are exactly eight such systems with h = 11 in the seminal paper,[10] the method was used to deduce the 98 and 1097 concealed non-Kekuléans with h = 12 and 13, respectively.[26] In the present work the method is applied to h = 14.

Basic Concepts. Let H be a benzenoid system (or hexagonal system) and adher to the convention that H is drawn in a plane so that some of its edges are vertical. The following concepts are taken from Sachs.[29]

A straight line segment C with end points P_1, P_2 is called a cut segment if (a) C is orthogonal to one of the three edge directions, (b) each P_1, P_2 is the center of an edge, (c) every point of C is either an interior or a boundary point of some hexagon of H, and (d) the graph obtained by deleting all the edges intersected by C has exactly two components.

Let C denote the set of edges intersected by a cut segment C of H. Assume that C is a horizontal single straight line segment, which is called a horizontal cut segment. Then C is called a horizontal cut of H. The two components of H-C are referred to as the upper and lower bank of H, denoted by U(C) and L(C), respectively.

A vertex of H which lies above (respectively below) all the vertices adjacent to it is called a peak (respectively valley) of H. The number of peaks (respectively valleys) of H is denoted by p(H) (respectively ν(H)). Finally, the numbers of peaks and valleys of H belonging to the upper bank are denoted by p(H/U(C)) and ν(H/U(C)), respectively.

Let Z denote the set of hexagons of H. For any S $\subset$ Z, we denote by H[S] the induced subgraph of S in H.

A concealed non-Kekuléan benzenoid shall presently be abbreviated to CNB.

Basic Theorems. The following theorem is crucial.

Theorem 1. Let H be a benzenoid system with h < 14. Then it has a Kekulé structure if and only if for every horizontal cut C in all the three possible directions

$$\text{(i) } p(\mathrm{H}) = \nu(\mathrm{H})$$

$$\text{(ii) } p(\mathrm{H/U(C)}) - \nu(\mathrm{H/U(C)}) \leq |\mathrm{C}|$$

The symbol |C| is used to designate the number of edges in C. A non-Kekuléan benzenoid which satisfies the conditions of theorem 1 must be a CNB and is said to be a CNB of type I. Furthermore, it must have $h \geq 14$. Theorem 1 is proved elsewhere,[10] as also is the following theorem.

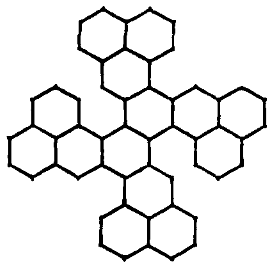

Figure 2. The smallest unique concealed non-Kekuléan benzenoid (CNB) of type I, H_I, which has $h = 14$.

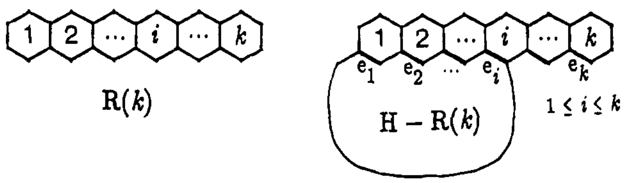

Figure 3. Illustration to the definition of a reducible benzenoid (cf.: definition 1).

Theorem 2. Let H be a smallest CNB of type I. Then

(i) H has $h = 14$

(ii) H is unique as shown in Figure 2

Let this system (Figure 2) be denoted by H_I.

Theorem 3. Let H be a CNB with $h < 14$. Then there is a horizontal cut C in H such that

$$\text{(i) } p(H/U(C)) - v(H/U(C)) > |C|$$

$$\text{(ii) } |C| = 2$$

This theorem is proved elsewhere.[26] Finally, we give a supplementary theorem for $h = 14$ below (without a formal proof).

Theorem 4. Let H be a CNB with $h = 14$ which is not H_I. Then there is a horizontal cut C in H such that

$$\text{(i) } p(H/U(C)) - v(H/U(C)) > |C|$$

$$\text{(ii) } |C| = 2 \text{ or } 3$$

Reducible and Irreducible Benzenoids. Because of the great complexity in enumerating all CNBs with $h = 14$, it is needed to extend the previously defined[26] concepts of reducible and irreducible benzenoid systems.

Definition 1. Let $R(k)$ denote the linear catacondensed benzenoid system (acene) with $k \geq 1$ hexagons (see left-hand part of Figure 3). If a benzenoid system H contains a subsystem $R(k)$ which is attached to the system induced by the other hexagons in H in the way as shown in the right-hand part of Figure 3, then H is said to be reducible, and the subsystem $R(k)$ is said to be a reducible part of H. If H contains no reducible part, it is said to be irreducible.

Assume that H is reducible with $R(k)$ as the reducible part. Then the system in H induced by the hexagons other than those in $R(k)$ is properly denoted by $H - R(k)$. It is convenient to say that H is obtained from $H' = H - R(k)$ by an *R*-operation to be indicated by $H = H' + R(k)$, and that H' is obtained from H by eliminating a reducible part, $R(k)$. If $k = 1$, the reducible part becomes a reducible hexagon, and our definitions coincide with those given previously.[26]

Property 1. Let $R(k)$ be a reducible part of a benzenoid system H. Then H is (concealed non-) Kekuléan if and only if $H - R(k)$ is (concealed non-) Kekuléan.

Let $R(i,j)$ denote the benzenoid system as shown in Figure 4a and $T(k)$ any catacondensed system with k hexagons. From definition 1 and property 1, we have the following corollary.

Corollary 1. Let $R(i,j)$ (respectively $T(k)$) be a subsystem in a benzenoid H which is attached to $H - R(i,j)$ (respectively $H - T(k)$) in the way as shown in Figure 4b (respectively Figure 4c). Then $R(i,j)$ (respectively $T(k)$) is a reducible part of H. Consequently, H is (concealed non-) Kekuléan if and only if $H - R(i,j)$ (respectively $H - T(k)$) is (concealed non-) Kekuléan.

Denote by N_h (respectively $\bar{N}_h$) the set of all reducible (respectively irreducible) CNBs with h hexagons. Then the set of all CNBs with h hexagons is $N_h \cup \bar{N}_h$.

Clearly, for any $H \in N_h$, in H there is a unique subsystem $H^* \in \bar{N}_{h-i}$, $1 \leq i \leq h - 11$, for which H can be constructed from H^* by some *R*-operations. Conversely, for any $H^* \in \bar{N}_{h-i}$, $1 \leq i \leq h - 11$, after some *R*-operations for which i hexagons are added to H^*, the resulting system H must belong to N_h. Consequently, N_{14} can be obtained recursively from $\bar{N}_{11} \cup \bar{N}_{12} \cup \bar{N}_{13}$.

For $\bar{N}_h$, $h \leq 14$, theorems 2 and 4 just offer the basis of a construction method.

Definition 2. Let H be a CNB in $\bar{N}_{14}$ which is not H_I. A horizontal cut C which satisfies the condition (i) in theorem 4 is said to be extremely up (respectively down) if in U(C) (respectively L(C)) there is no other horizontal cut satisfying (i).

Denote by C_u and C_d the extremely up and down horizontal cuts, respectively (possibly $C_u = C_d$). Further, denote by X and Y the sets of hexagons in $U(C_u)$ and $L(C_d)$, respectively, when referring to the upper and lower bank. Denote also by W_u (respectively W_d) the set of hexagons which contain the edges in C_u (respectively C_d). Now $H[Z \backslash X \cup Y]$ is adequately called the link between $U(C_u)$ and $L(C_d)$, and it is denoted by L_i, where i is the number of hexagons in the link.

When we give all possible $U(C_u)$, L_i, and $L(C_d)$, we shall be able to enumerate combinatorially all CNBs in $\bar{N}_{14}$.

Theorem 5. Assume that $H \in \bar{N}_h$, $h \leq 14$, and that H is not H_I. Let C_u (respectively C_d) be the extremely up (respectively down) horizontal cut of H satisfying

$$p(H/U(C_u)) - v(H/U(C_u)) > |C_u|$$

$$(\text{respectively } p(H/U(C_d)) - v(H/U(C_d)) > |C_d|)$$

Then $H[X \cup W_u]$ (respectively $H[Y \cup W_d]$) must be isomorphic to one of the benzenoid systems as shown in Figures 5 and 6 and L_i must be isomorphic to one of the benzenoids as shown in Figure 7.

Now we are in position to enumerate all nonisomorphic CNBs with $h = 14$.

Enumeration of All Concealed Non-Kekuléan Benzenoids with Fourteen Hexagons. For the systems in Figures 5 and 6, introduce the notations $A = \{A_1, A_2, A_3\}$,

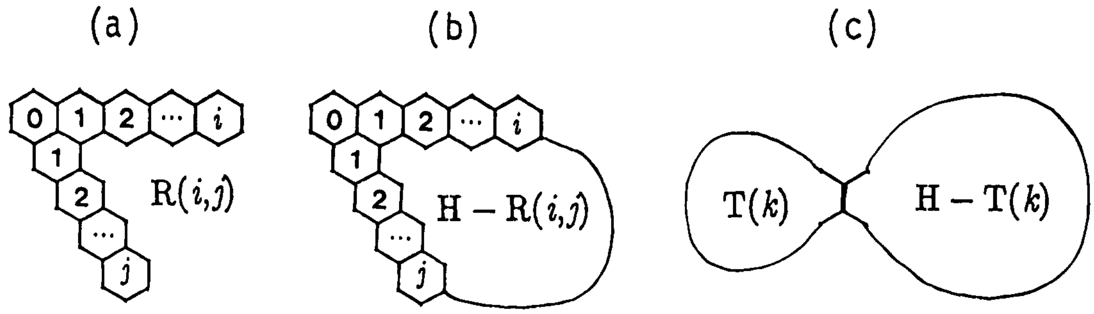

Figure 4. Illustration to corollary 1.

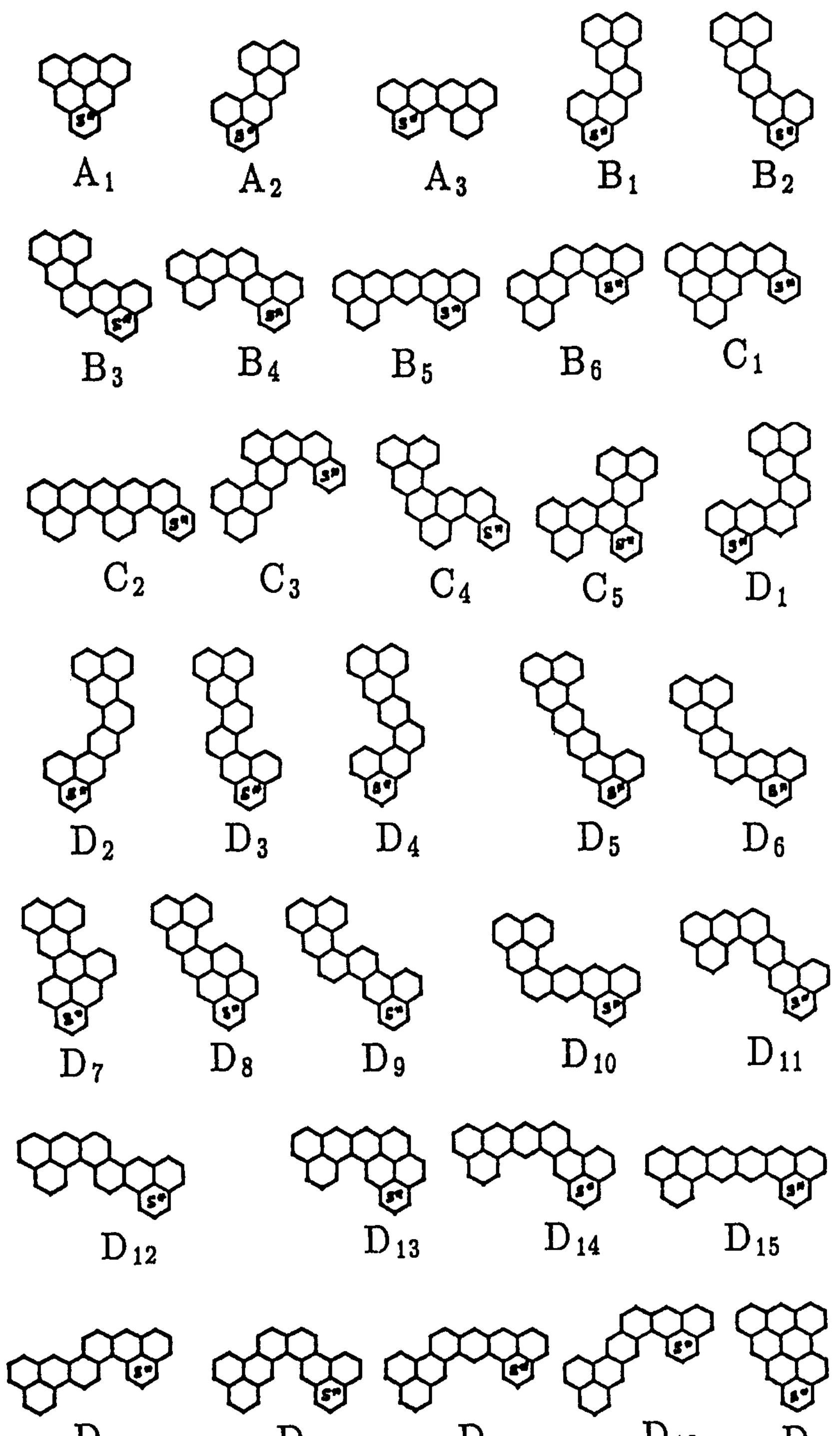

Figure 5. Fragments of $h = 14$ concealed non-Kekuléan benzenoids, which can be linked at the marked hexagons.

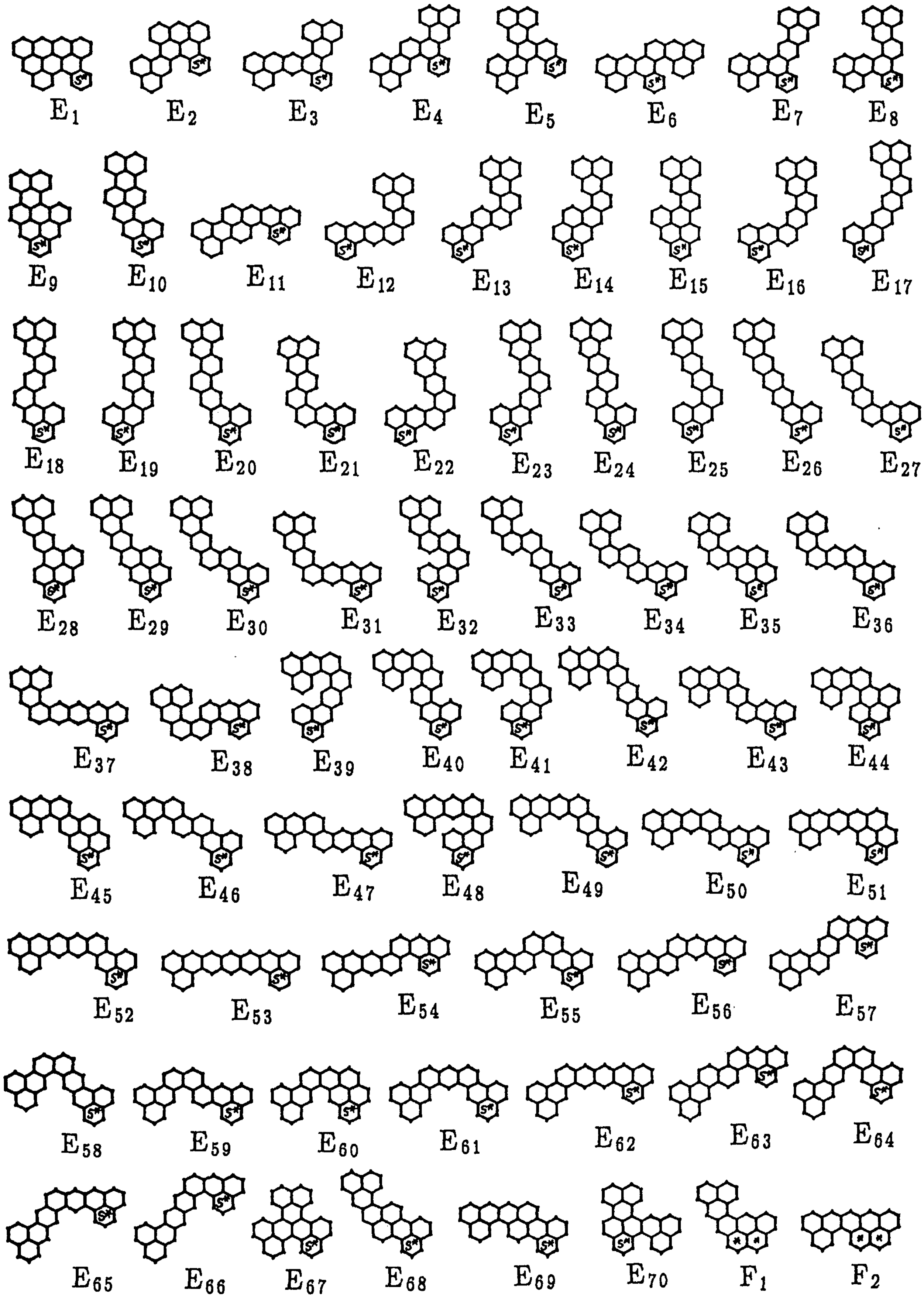

Figure 6. Fragments of $h = 14$ concealed non-Kekuléan benzenoids, which can be linked at the marked hexagons.

$B = \{B_1, B_2, ..., B_6\}$, $C = \{C_1, C_2, ..., C_5\}$, $D = \{D_1, D_2, ..., D_{20}\}$, $E = \{E_1, E_2, ..., E_{70}\}$, and $F = \{F_1, F_2\}$. Assume that $P, Q \in \{A, B, C, D, E, F\}$, $N' \subset P$, and $N'' \subset Q$. Furthermore, let $\bar{N}_h(N', L_i, N'') \subset \bar{N}_h$, $h \leq 14$, be the set of all the CNBs for which $H \in \bar{N}_h(N', L_i, N'')$ if $H[X \cup W_u]$ (respectively $H[Y \cup W_d]$) is isomorphic to a system in N' (respectively N''), and $H[Z \backslash X] \cup Y]$ is isomorphic to a system in L_i.

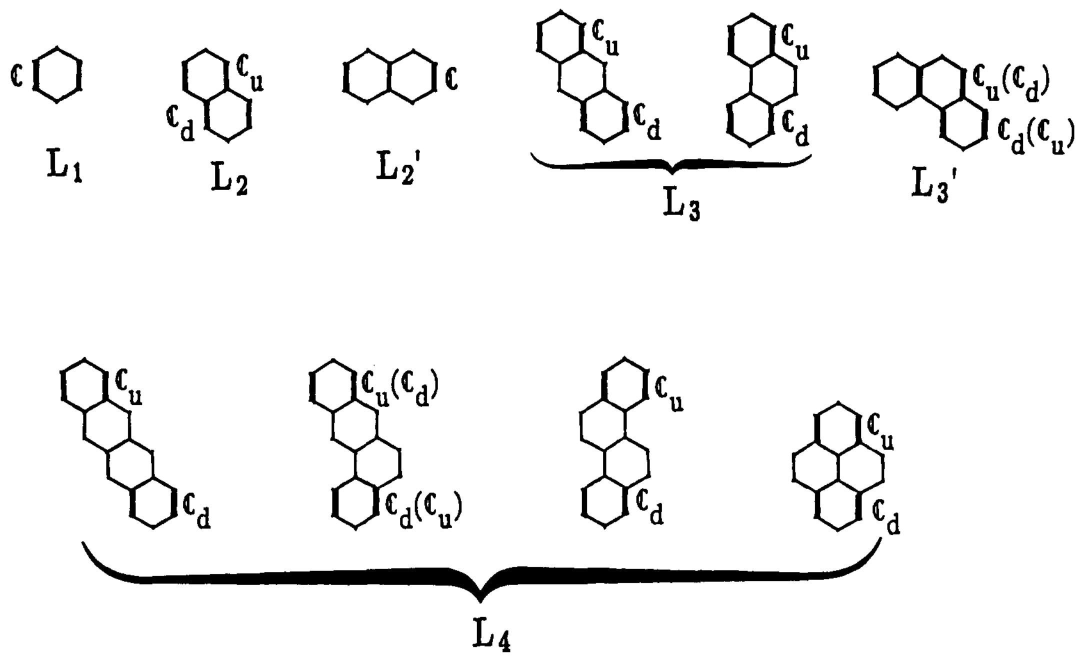

Figure 7. Links of $h = 14$ concealed non-Kekuléan benzenoids.

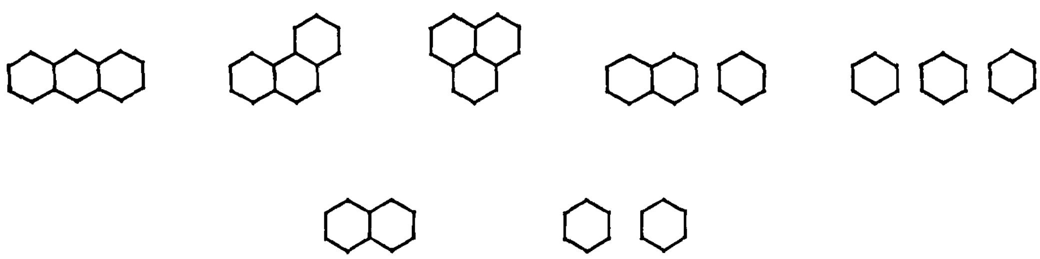

Figure 8. Reducible parts of $h = 14$ concealed non-Kekuléan benzenoids.

It is found for the relevant numbers

$$|\bar{N}_{14}(A, L_4, A)| = 74$$

$$|\bar{N}_{14}(A, L_3, B)| = 117$$

$$|\bar{N}_{14}(A, L_2, C \cup D)| = 234$$

$$|\bar{N}_{14}(A, L_1, E)| = 312$$

$$|\bar{N}_{14}(A, L_3', F)| = 8$$

$$|\bar{N}_{14}(B, L_2, B)| = 71$$

$$|\bar{N}_{14}(B, L_1, C \cup D)| = 252$$

$$|\bar{N}_{14}(F, L_2', F)| = 5$$

$$\{H_I\}| = 1$$

Consequently,

$$|\bar{N}_{14}| = 74 + 117 + 234 + 312 + 8 + 71 + 252 + 5 + 1 = 1074$$

It remains to enumerate the systems in N_{14}.

Let $N_h(\bar{N}_{h-i})$, $1 \le i \le h - 11$, denote the set of the systems in N_h, each of which is obtained from a system in $\bar{N}_{h-i}$ by some R-operations. For $H \in N_h(\bar{N}_{h-i})$, let H^* denote the corresponding system in $\bar{N}_{h-i}$, Z^* the set of hexagons in H^*; then $H[Z\backslash Z^*]$ are the reducible parts of H. For $H \in N_{14}(\bar{N}_{11})$, $H[Z\backslash Z^*]$ is isomorphic to one of the five graphs in the top row of Figure 8. For $H \in N_{14}(\bar{N}_{12})$, $H[Z\backslash Z^*]$ is isomorphic to one of the two graphs in the bottom row of Figure 8. Finally, for $H \in N_{14}(\bar{N}_{13})$, $H[Z\backslash Z^*]$ is only one hexagon.

A systematic enumeration leads to the following results.

$$|N_{14}(\bar{N}_{11})| = 2775$$

$$|N_{14}(\bar{N}_{12})| = 3418$$

$$|N_{14}(\bar{N}_{13})| = 2537$$

Consequently,

$$|N_{14}| = 2775 + 3418 + 2537 = 8730$$

The net result is

$$|N_{14} \cup \bar{N}_{14}| = 8730 + 1074 = 9804$$

Theorem 6. There are exactly 9804 CNBs with $h = 14$.

CONCLUSION

The above application of the construction method[10] for concealed non-Kekuléan benzenoids is supposed to demonstrate the virtue of this method.[30] The number in theorem 6 is identical with the corresponding number from computer programming (cf. Table 1). Hereby the controversy which was mentioned in the Introduction is definitely resolved.

Table 4. Numbers of C_nH_s Isomers of Concealed Non-Kekuléan Helicenes

	n_i			
h	4	6	8	total
11	1			1[a]
12	16	1		17[a]
13	240	28	1	269[a]

[a] Zhang and Guo (1992).[31]

Furthermore, the confidence in the higher numbers (for $h > 14$) in Table 1 is strengthened. It is supposed that the present work is the last word in the general search for concealed non-Kekuléan benzenoids, which started with two systems[4] in 1974. It seems not warranted to pursue this search further, since no fundamentally new properties of still larger such systems are expected.

APPENDIX: CONCEALED NON-KEKULEAN HELICENES

In a recent work, Zhang and Guo[31] applied the construction method to concealed non-Kekuléan helicenes.[13] They found the numbers 1, 17, and 269 for h = 11, 12, and 13, respectively, and concluded by saying that it would have been interesting to check these numbers by computer programming. An extensive computerized enumeration of helicenes has now been completed, and it confirms the above numbers. Relevant results from these computations are shown in Table 4, where the classification according to the number of internal vertices is included. This is virtually an enumeration of a certain class of C_nH_s isomers; the appropriate formulas form a subset of the benzenoid formulas and are found in Table 2.

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