Mono-Q-Polyhexes with Q Larger than 6: Polygonal Systems Representing a Class of Polycyclic Conjugated Hydrocarbons

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Mono-Q-fusenes are simply connected mono-Q-polyhexes, consisting of exactly one Q-gon in addition to only hexagons (if any). Mono-Q-benzenoids are geometrically planar (non-helicenic) mono-Q-fusenes. Extensive enumerations of the C_nH_s isomers of monooctabenzenoids ($Q = 8$) are reported and the forms of the smallest of these systems (up to four hexagons) are depicted. The properties of extremal mono-Q-benzenoids for $Q > 6$ are studied in detail. These systems are defined in analogy with the extremal mono-q-benzenoids for $q < 6$, but are found to exhibit largely different properties, especially with respect to circumscribing. Some results are also reported from enumerations of the extremal mono-Q-benzenoids. Especially for circular mono-Q-benzenoids, a subclass of the extremal systems, a complete mathematical solution of the enumeration problem was achieved.

INTRODUCTION

Completely condensed polycyclic conjugated hydrocarbons[1,2] are of great interest in organic, physical, and mathematical chemistry. As chemical graphs[3] they are represented by polygonal systems, viz. connected geometrical constructions of polygons, where any two polygons either share exactly one edge or are disjointed. Dias[2,4] considered in particular the systems with hexagons and/or polygons of one definite size. A mono-q-polyhex[5] is a polygonal system consisting of exactly one q-gon and otherwise hexagons (if any). The biphenylenoids[6] correspond to monotetrapolyhexes ($q = 4$). Fluoranthenoids and fluorenoids[7-9] are represented by monopentapolyhexes ($q = 5$), to which the interesting $C_{20}H_{10}$ structure pentacirculene (corannulene)[10-13] belongs. Benzenoids[1,2,14] are simply polyhexes, i.e. mono-q-polyhexes with $q = 6$. Hexacirculene ($C_{24}H_{12}$), for instance, is the well-known coronene.[1,15] The amount of work which has been done on the topological properties of benzenoids is formidable. In addition, some general formulations for mono-q-polyhexes when $q < 6$ are available.[6,16] Much less work has been done on mono-q-polyhexes when $q > 6$. Nevertheless, seven-membered rings are abundant among the polycyclic conjugated hydrocarbons, and such an interesting $C_{28}H_{14}$ structure as heptacirculene[17] belongs to monoheptapolyhexes ($q = 7$). Some enumerations of monoheptabenzenoids (a class of monoheptapolyhexes) are available, along with some theoretical considerations,[18] which are rather fragmentary. The topological properties of mono-q-polyhexes are substantially different whether $q < 6$ or $q > 6$, as might be expected. It is warranted, in fact, to change the notation to mono-Q-polyhex when $Q > 6$, while the term mono-q-polyhex may be reserved for the case of $q < 6$.

Also the eight-membered conjugated rings are abundant among chemical structures.[1,2,4] The main subject of the present work are the monooctapolyhexes ($Q = 8$). Among the chemical counterparts are, for instance, $C_{32}H_{16}$ octacirculene[19] and $C_{24}H_{16}$ tetraphenylene;[1] see Figure 1. The present work includes a number of new general formulations for mono-Q-polyhexes ($Q > 6$).

Circumscribing is a well-known concept in organic chemistry.[1] Its importance in a special context has been pointed out by Dias,[2] and it is also crucial in the present theory.

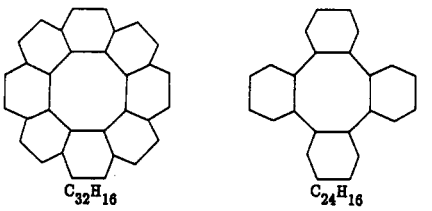
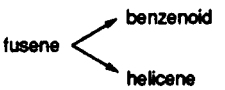


Figure 1. Two representatives of monooctapolyhexes.

BASIC CONCEPTS

Definitions and Terminology. In this work only simply connected polygonal systems are considered; i.e. they should not have any holes. A simply connected mono-Q-polyhex is called mono-Q-fusene and identified by the symbol M_Q. It is assumed that $Q > 6$. A mono-Q-fusene may be geometrically planar (nonhelicenic) or geometrically nonplanar (helicenic), referred to as mono-Q-benzenoid or mono-Q-helicene, respectively. This classification is compatible with the classification of simply connected polyhexes according to:[20]



It is adhered to one of the usual definitions of benzenoids.[14] In consequence, a mono-Q-benzenoid may be defined by a cycle on the mono-Q-hexagonal lattice.[5] An example for a monooctabenzenoid is shown in Figure 2.

Invariants and Functions of Invariants. The number of hexagons in a mono-Q-fusene (M_Q) is denoted by h; one may have $h = 0, 1, 2, \ldots$, where $h = 0$ pertains to the Q-gon alone. The total number of polygons is $h + 1$. The number of internal vertices is n_i.

The chemical formula of M_Q, viz., $C_nH_s \equiv (n; s)$, contains other important invariants (in addition to h and n_i): the total number n of vertices and the number s of the vertices of degree 2. One has

$$h = {}^1/_2(n - s), \quad n_i = n - 2s + Q \tag{1}$$

$$(n; s) = (4h - n_i + Q; 2h - n_i + Q) \tag{2}$$

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Table 1. Formulas for Monooctafusenes

	n_i										
h	0	1	2	3	4	5	6	7	8	9	10
0	C_8H_8										
1	$C_{12}H_{10}$										
2	$C_{16}H_{12}$	$C_{15}H_{11}$									
3	$C_{20}H_{14}$	$C_{19}H_{13}$	$C_{18}H_{12}$								
4	$C_{24}H_{16}$	$C_{23}H_{15}$	$C_{22}H_{14}$	$C_{21}H_{13}$							
5	$C_{28}H_{18}$	$C_{27}H_{17}$	$C_{26}H_{16}$	$C_{25}H_{15}$	$C_{24}H_{14}$						
6	$C_{32}H_{20}$	$C_{31}H_{19}$	$C_{30}H_{18}$	$C_{29}H_{17}$	$C_{28}H_{16}$	$C_{27}H_{15}$	$C_{26}H_{14}$				
7	$C_{36}H_{22}$	$C_{35}H_{21}$	$C_{34}H_{20}$	$C_{33}H_{19}$	$C_{32}H_{18}$	$C_{31}H_{17}$	$C_{30}H_{16}$	$C_{29}H_{15}$			
8	$C_{40}H_{24}$	$C_{39}H_{23}$	$C_{38}H_{22}$	$C_{37}H_{21}$	$C_{36}H_{20}$	$C_{35}H_{19}$	$C_{34}H_{18}$	$C_{33}H_{17}$	$C_{32}H_{16}$		
9	$C_{44}H_{26}$	$C_{43}H_{25}$	$C_{42}H_{24}$	$C_{41}H_{23}$	$C_{40}H_{22}$	$C_{39}H_{21}$	$C_{38}H_{20}$	$C_{37}H_{19}$	$C_{36}H_{18}$	$C_{35}H_{17}$	$C_{34}H_{16}$

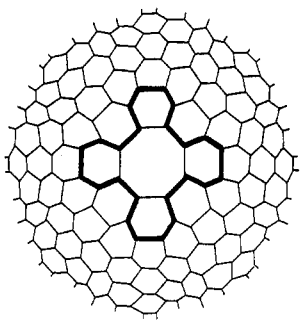

Figure 2. Tetraphenylene ($C_{24}H_{16}$) defined by its perimeter, a cycle on the monooctahexagonal lattice.

The symbol $M_Q(n;s)$ is used to indicate that M_Q has the formula (n; s). Two nonisomorphic systems M_Q and M_Q' with a given Q are said to be isomers when they have the same formula: $M_Q(n;s)$, $M_Q'(n;s)$.

Assume that $M_Q(n;s)$ can be circumscribed by s hexagons, and set circum-$M_Q(n;s)$ = (circum-M_Q)$(n_1;s_1)$. Then

$$(n_1; s_1) = (n + 2s + Q; s + Q) \quad (3)$$

Example (see Figure 1): circum-C_8H_8 = $C_{32}H_{16}$. The generalization of eq 3 for k-fold circumscribing reads

$$(n_k; s_k) = (n + 2ks_0 + k^2Q; s_0 + kQ) \quad (4)$$

Here k-circum-$M_Q(n_0;s_0)$ = (k-circum-M_Q)$(n_k;s_k)$. All the relations of eqs 1–4 have the same forms as the corresponding relations for mono-q-fusenes[6] with $q < 6$. The functions $(n_i)_{max}$-(h), $h_{max}(s)$, $n_{max}(s)$, and $s_{min}(n)$, on the other hand, are substantially different for M_Q and M_q. These functions (for M_Q) are found among the inequalities in the following.

For n_i of M_Q it was found[18]

$$0 \le n_i \le 2h + 3 - \lceil (12h + 9)^{1/2} \rceil \quad (5)$$

independent of Q. The number n_i of internal vertices may in general assume any positive integer value but is limited upward for a given h. Here, we give for the first time the relation

$$0 \le h \le \lfloor {}^1/_{12}(s - Q)(s - Q + 6) \rfloor \quad (6)$$

which was found for M_Q and implies the maximum value of h for a given s.

For a given n, which C_nH_s formulas are possible for mono-Q-fusenes? The answer is given by

$$2\lceil {}^1/_2(n - Q) + {}^1/_2(6^{1/2})(n - Q + 6)^{1/2} \rceil - n + 2Q - 6 \le s \le n - 2\lceil {}^1/_4(n - Q) \rceil \quad (7)$$

where $n = Q$, $Q + 4$, $Q + 7$, $Q + 8$, or $n \ge Q + 10$. We have also found the answer to the question: for a given s, which C_nH_s formulas are possible for mono-Q-fusenes?

$$s + 2\lceil {}^1/_2(s - Q) \rceil \le n \le s + 2\lfloor {}^1/_{12}(s - Q)(s - Q + 6) \rfloor \quad (8)$$

where $s = Q$ or $s \ge Q + 2$. In both eqs 7 and 8 the upper and lower bounds are always realized for M_Q in general, but the parities must be taken into account: either both n and s are even, or both of them are odd. The bounds of eqs 7 and 8 are the best possible "sharp bounds" in the sense of Hansen and Zheng.[21]

The smallest chemical formulas (C_nH_s) for monooctafusenes, the same as for monooctabenzenoids, are listed in Table 1. The table extends infinitely downward, while each row becomes longer and longer.

A one-to-one correspondence exists between all the possible C_nH_s mono-Q-fusene/mono-Q-benzenoid formulas and all the possible C_NH_S fusene/benzenoid formulas:

$$n = N + Q - 6, \quad s = S + Q - 6 \quad (9)$$

Any hexagon at the perimeter of a fusene B can be expanded to a Q-gon, in analogy with the hexagon-to-pentagon contraction of Dias.[7] If $B(N;S)$ is modified in this way, the resulting mono-Q-fusene, for example, $B'(n;s)$, acquires its formula (n; s) in accordance with eq 9. Furthermore, it is inferred that this conversion $C_NH_S \rightarrow C_nH_s$ accounts for all the possible mono-Q-fusene/mono-Q-benzenoid formulas.

Classes. Some classes of mono-Q-fusenes are defined in analogy with corresponding classes of fusenes.[14,20,22,23] The corresponding classification has also been defined for mono-q-fusenes.

A mono-Q-fusene is catacondensed for $n_i = 0$, pericondensed for $n_i > 0$. An extremal mono-Q-fusene is defined by having the maximum number n_i of internal vertices for a given number h of hexagons: $n_i = (n_i)_{max}(h)$. A mono-Q-fusene which is not extremal is called nonextremal. An extremal mono-Q-fusene is always a mono-Q-benzenoid. The circular mono-Q-benzenoids form a subclass of the extremal mono-Q-benzenoids and are defined by having the maximum number h of hexagons for a given perimeter length or s value: $h = h_{max}(s)$. A mono-Q-fusene which is not circular is called noncircular.

COMPUTERIZED ISOMER ENUMERATION

The first systematic enumerations of mono-Q-benzenoids were reported for the monoheptabenzenoids ($Q = 7$).[18] A corresponding study for $Q = 8$ is described in the following.

A computer program was designed in order to generate the monooctabenzenoids C_nH_s isomers with increasing h values. Monooctahelicenes are not included. A complete listing of the numbers of isomers for $h \le 7$ is given in Table 2, while Table 3 shows incomplete data for higher h values, but so that

Table 2. Numbers of Nonisomorphic C_nH_s Isomers of Simply Connected, Geometrically Planar Monooctapolyhexes (Monooctabenzenoids): Complete Data for $h \leq 7$

h	n_i	formula	D_{8h}	D_{4h}(a)	D_{2h}(a)	D_{2h}(b)	C_{2h}	C_{2v}(a)	C_{2v}(b)	C_s	total
0	0	C_8H_8	1	0	0	0	0	0	0	0	1
1	0	$C_{12}H_{10}$	0	0	0	0	0	1	0	0	1
2	0	$C_{16}H_{12}$	0	0	1	0	0	2	1	1	5
	1	$C_{15}H_{11}$	0	0	0	0	0	0	1	0	1
3	0	$C_{20}H_{14}$	0	0	0	0	0	5	0	11	16
	1	$C_{19}H_{13}$	0	0	0	0	0	0	0	5	5
	2	$C_{18}H_{12}$	0	0	0	0	0	1	1	0	2
4	0	$C_{24}H_{16}$	0	1	1	0	1	10	3	56	72
	1	$C_{23}H_{15}$	0	0	0	0	0	0	3	34	37
	2	$C_{22}H_{14}$	0	0	0	1	0	4	0	9	14
	3	$C_{21}H_{13}$	0	0	0	0	0	0	1	2	3
5	0	$C_{28}H_{18}$	0	0	0	0	0	20	0	279	299
	1	$C_{27}H_{17}$	0	0	0	0	0	0	0	218	218
	2	$C_{26}H_{16}$	0	0	0	0	0	10	2	87	99
	3	$C_{25}H_{15}$	0	0	0	0	0	0	2	27	29
	4	$C_{24}H_{14}$	0	0	0	0	0	2	2	5	9
6	0	$C_{32}H_{20}$	0	0	3	0	5	42	10	1269	1329
	1	$C_{31}H_{19}$	0	0	0	0	0	0	10	1217	1227
	2	$C_{30}H_{18}$	0	0	0	0	3	29	6	643	681
	3	$C_{29}H_{17}$	0	0	0	0	0	0	4	240	244
	4	$C_{28}H_{16}$	0	0	1	1	0	5	2	77	86
	5	$C_{27}H_{15}$	0	0	0	0	0	0	2	17	19
	6	$C_{26}H_{14}$	0	0	0	0	0	1	0	0	1
7	0	$C_{36}H_{22}$	0	0	0	0	0	76	0	5728	5804
	1	$C_{35}H_{21}$	0	0	0	0	0	0	0	6502	6502
	2	$C_{34}H_{20}$	0	0	0	0	0	62	7	4191	4260
	3	$C_{33}H_{19}$	0	0	0	0	0	0	6	1845	1851
	4	$C_{32}H_{18}$	0	0	0	0	0	18	6	708	732
	5	$C_{31}H_{17}$	0	0	0	0	0	0	4	218	222
	6	$C_{30}H_{16}$	0	0	0	0	0	7	4	44	55
	7	$C_{29}H_{15}$	0	0	0	0	0	0	1	3	4

Table 3. Numbers of Nonisomorphic C_nH_s Isomers of Simply Connected, Geometrically Planar Monooctapolyhexes (Monooctabenzenoids): Incomplete Data for $8 \leq h \leq 15$

h	n_i	formula	D_{8h}	D_{2h}(b)	C_{2h}	C_{2v}(a)	C_{2v}(b)	C_s	total
8	5	$C_{35}H_{19}$	0	0	0	0	12	2052	2064
	6	$C_{34}H_{18}$	0	0	2	19	6	606	633
	7	$C_{33}H_{17}$	0	0	0	0	4	136	140
	8	$C_{32}H_{16}$	1	0	0	3	1	16	21
9	7	$C_{37}H_{19}$	0	0	0	0	10	1705	1715
	8	$C_{36}H_{18}$	0	0	0	18	6	418	442
	9	$C_{35}H_{17}$	0	0	0	0	3	66	69
	10	$C_{34}H_{16}$	0	0	0	1	1	1	3
10	9	$C_{39}H_{19}$	0	0	0	0	13	1308	1321
	10	$C_{38}H_{18}$	0	1	0	13	5	220	239
	11	$C_{37}H_{17}$	0	0	0	0	0	18	18
11	11	$C_{41}H_{19}$	0	0	0	0	11	758	769
	12	$C_{40}H_{18}$	0	0	0	6	3	95	104
	13	$C_{39}H_{17}$	0	0	0	0	1	1	2
12	13	$C_{43}H_{19}$	0	0	0	0	2	407	409
	14	$C_{42}H_{18}$	0	0	0	3	2	20	25
13	15	$C_{45}H_{19}$	0	0	0	0	6	154	160
	16	$C_{44}H_{18}$	0	0	0	1	0	2	3
14	17	$C_{47}H_{19}$	0	0	0	0	1	38	39
15	19	$C_{49}H_{19}$	0	0	0	0	1	5	6

the extremal systems for every $h \leq 15$ are included. A special algorithm was used to recognize the symmetry of the generated systems. In general, the possible symmetry groups are D_{8h}, C_{8h}, D_{4h}, C_{4h}, D_{2h}, C_{2h}, C_{2v}, and C_s. A finer classification for some of these symmetry groups is useful: one distinguishes the types D_{2h}(a) and D_{2h}(b) when the two-fold symmetry axes (a) intersect edges in the octagon or (b) pass through some of its vertices, respectively. Similarly, C_{2v}(a) and C_{2v}(b) pertain to the cases when the 2-fold symmetry axis (a) intersects two edges in the octagon or (b) passes through two of its vertices. The symmetry distributions are included in Tables 2 and 3. Herein there are no entries for C_{8h}, D_{4h}(b), and C_{4h}. The smallest C_{8h} monooctapolyhex (monooctabenzenoid) has $h = 24$, while D_{4h}(b) first occurs at $h = 12$, and

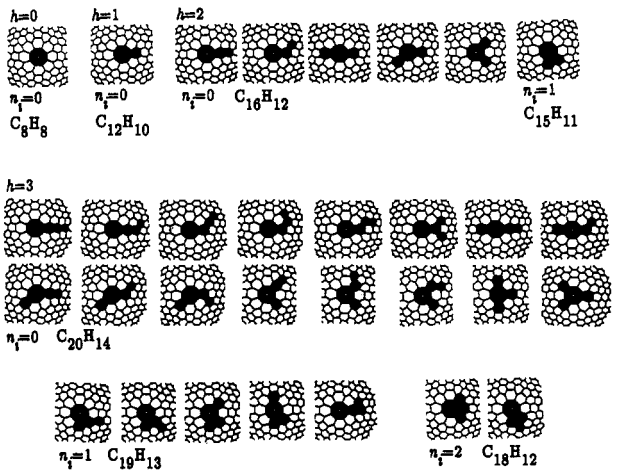

Figure 3. All nonisomorphic monooctafusenes (which are monooctabenzenoids) for $h \leq 3$, represented as black silhouettes on the background of the monooctahexagonal lattice. The octagon is marked by a white dot.

C_{4h} already by a unique catacondensed system at $h = 8$.

The smallest ($h \leq 4$) forms of the monooctabenzenoids are depicted in Figures 3–5. They were generated by hand but checked against the numbers and symmetries from the computer results.

EXTREMAL SYSTEMS

Principles of Generation. Denote an extremal benzenoid by $A(N^a;S^a)$. On expanding one of the hexagons at the perimeter of A to a Q-gon, an extremal mono-Q-benzenoid, for example, $A_Q(n^a;s^a)$ emerges. In this way there is a one-to-one correspondence between the formulas $(N^a;S^a)$ of all A benzenoids and the formulas $(n^a; s^a)$ of A_Q. This does not imply, however, that all isomers of A_Q are generated by the described process. As we shall find, it happens exceptionally

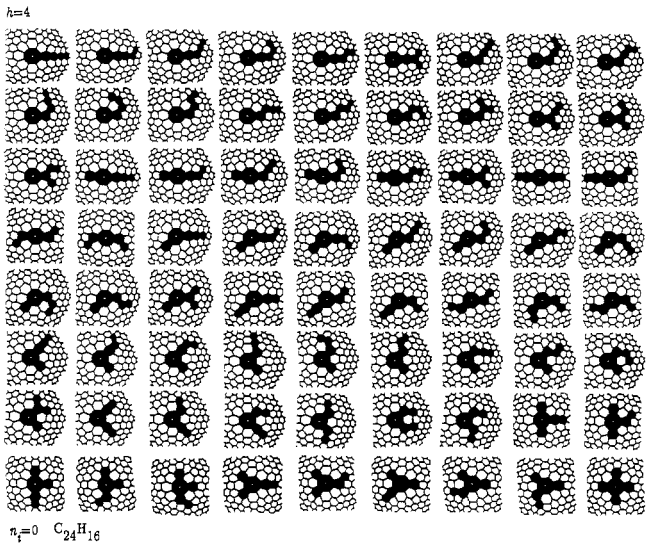

Figure 4. Nonisomorphic catacondensed monooctafusenes (monooctabenzenoids) for $h = 4$.

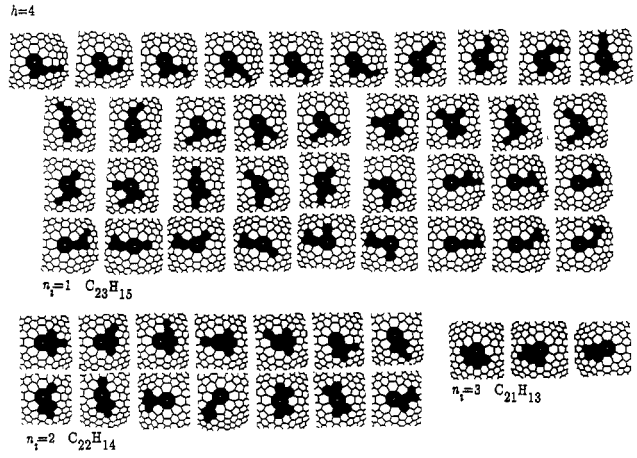

Figure 5. Nonisomorphic pericondensed monooctafusenes (monooctabenzenoids) for $h = 4$.

that an A_Q isomer has its Q-gon completely surrounded by hexagons. Very exceptionally, actually in a unique A_Q system, the 2-fold circumscribed Q-gon is a subgraph of A_Q.

It is emphasized that the spiral walk[24,25] does not in general produce extremal mono-Q-benzenoids. Notice that, if a system S is generated during the spiral walk, then circum-S will eventually be produced on continuing the same process. The spiral walk generates extremal benzenoids,[24,25] extremal monopentabenzenoids,[8] and other mono-q-benzenoids[6] ($q < 6$). On the other hand, extremal mono-q-benzenoids are not obtained in general by the procedure described above for mono-Q-benzenoids ($Q > 6$). The reader is referred to additional recent studies which have been made on extremal benzenoids.[26-28]

Chemical Formulas. For an extremal mono-Q-benzenoid, $A_Q(n^a;s^a)$, it is readily found from eqs 2 and 5:

$$(n^a; s^a) = (2h + Q - 3 + \lceil(12h + 9)^{1/2}\rceil; Q - 3 + \lceil(12h + 9)^{1/2}\rceil) \quad (10)$$

This equation is valid for benzenoids on inserting $Q = 6$ only if h simultaneously is redefined as one unit less than the number of hexagons. The first ten A_Q systems (for $Q \geq 6$) have the following formulas: C_QH_Q, $C_{Q+4}H_{Q+2}$, $C_{Q+7}H_{Q+3}$, $C_{Q+10}H_{Q+4}$, $C_{Q+13}H_{Q+5}$, $C_{Q+16}H_{Q+6}$, $C_{Q+18}H_{Q+6}$, $C_{Q+21}H_{Q+7}$, $C_{Q+24}H_{Q+8}$, and $C_{Q+26}H_{Q+8}$. The formulas for extremal monooctabenzenoids ($Q = 8$) are found at the extreme right of each row in the listing of formulas in the representation of Table 1.

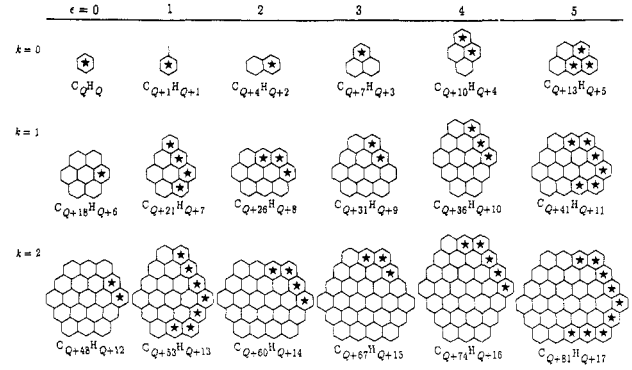

Figure 6. Circular benzenoids (including one degenerate system, the non-benzenoid C_7H_7), and their conversion to circular mono-Q-benzenoids. See the text for explanation.

For a circular mono-Q-benzenoid, for example, $O_Q(n^O;s^O)$, it is readily found from eqs 1 and 6:

$$(n^O; s^O) = (s + 2\lfloor{}^1/_{12}(s - Q)(s - Q + 6)\rfloor; s) \quad (11)$$

The possible values of $s = s^O$ are given under eq 8. Relation 11 is valid for benzenoids with $Q = 6$. Another approach to the O_Q systems is useful. Consider the circular benzenoids $O(N^O;S^O)$, which are known to have six characteristic forms.[29,30] For the sake of convenience the smallest O systems are depicted in Figure 6. All the larger O systems are obtained on successive circumscribings. The systems O are converted to O_Q by expanding the hexagons at their perimeters, one at a time, to Q-gons. If the hexagons marked with asterisks in Figure 6 are expanded, one at a time, sets of nonisomorphic O_Q systems are generated. It is not claimed (and actually not true, as we shall see) that all isomers O_Q are generated in this way, but all $(n^O; s^O)$ formulas are covered. Now we have[23,30]

$$(N^O; S^O) = (S + \lfloor{}^1/_{12}(S^2 - 6S)\rfloor; S) \quad (12)$$

for the circular benzenoids $O(N^O;S^O)$. Here $S = 6$ and $S \geq 8$ if the degenerate system C_7H_7 is excluded. From eq 9, which reflects the described expansion from hexagon to Q-gon, one obtains for the circular mono-Q-benzenoids

$$(n^O; s^O) = (S + Q - 6 + 2\lfloor{}^1/_{12}(S^2 - 6S)\rfloor; S + Q - 6) \quad (13)$$

This relation indeed becomes identical with eq 11 on substituting $s = S + Q - 6$.

Criterion. On inserting into eq 5 from 1 it is obtained

$$\lceil(6n - 6s + 9)^{1/2}\rceil \leq s - Q + 3 \quad (14)$$

for a mono-Q-fusene. This relation is convenient for deciding directly whether $M_Q(n;s)$ is an extremal or nonextremal mono-Q-fusene. The sign of equality in eq 14 is valid if and only if M_Q is extremal, i.e.

$$\lceil(6n^a - 6s^a + 9)^{1/2}\rceil = s^a - Q + 3 \quad (15)$$

This is the criterion for $A_Q(n^a;s^a)$ to be extremal. Relations 14 and 15 are also valid for fusenes on inserting $Q = 6$; in other words,

$$\lceil(6N - 6S + 9)^{1/2}\rceil \leq S - 3 \quad (16)$$

decides whether $B(N;S)$ is an extremal or nonextremal fusene. The system $A(N^a;S^a)$ is an extremal benzenoid if and only if

$$\lceil (6N^a - 6S^a + 9)^{1/2} \rceil = S^a - 3 \quad (17)$$

It is implied in the above discussion that all the formulas for $A_Q(n^a;s^a)$ are obtained as $(N^a + Q - 6; S^a + Q - 6)$ when $(N^a; S^a)$ represents the formulas for extremal benzenoids. Similarly, all the formulas for $O_Q(n^O;s^O)$ are obtained as $(N^O + Q - 6; S^O + Q - 6)$ when $(N^O; S^O)$ represent the formulas for circular benzenoids. Furthermore, if $B(N;S)$ is nonextremal (noncircular), then also $M_Q(N + Q - 6; S + Q - 6)$ will be nonextremal (noncircular).

Properties with Respect to Circumscribing. The following properties have been proved for benzenoids.[25-28] (a) Any extremal benzenoid can be circumscribed arbitrarily many times. (b) Among the benzenoid isomers with any formula C_NH_S there is at least one isomer which can be circumscribed arbitrarily many times. (c) A circumscribed extremal benzenoid is itself an extremal benzenoid. The corresponding three properties are also valid for mono-q-benzenoids[5] (mono-q-fusenes) with $q < 6$, and the two first properties, a and b, also for mono-Q-benzenoids (mono-Q-fusenes) with $Q > 6$. In sharp contrast, property c is not valid for the systems with $Q > 6$, as already is implied in the above discussions.

Assume the transformation of formulas $(N; S) \rightarrow (N + Q - 6; S + Q - 6)$, which corresponds to the modification of $B(N;S)$ by expanding one of its hexagons at the perimeter to a Q-gon: $B \rightarrow B'$. Furthermore, consider the formula which corresponds to k-fold circumscribed B′, viz. k-circum-B′, and designate it $(n_k'; s_k')$. Then, by means of eq 4 it is obtained

$$(n'_k; s'_k) = (N + 2kS + (k+1)^2Q - 6(2k+1); S + (k+1)Q - 6) \quad (18)$$

Lemma 1. If $M_Q(n_k';s_k')$ is a nonextremal mono-Q-fusene for a certain Q, then $M_{Q'}$ will also be nonextremal if $Q' > Q$.

Proof. Apply the criterion 14 to $(n_k'; s_k')$ from eq 18. It gives

$$\lceil [6N + 6(2k-1)S + 6k(k+1)Q - 72k + 9]^{1/2} \rceil < S + kQ - 3 \quad (19)$$

A general condition for an integer A reads $A > \lceil x \rceil$ if and only if $A \geq x + 1$. Hence

$$[6N + 6(2k-1)S + 6k(k+1)Q - 72k + 9]^{1/2} + 1 \leq S + kQ - 3 \quad (20)$$

Elementary manipulations of eq 20 gave the following equivalent relation.

$$6N - S^2 + 2(6k+1)S - 72k - 7 \leq k^2Q^2 + 2k(S - 3k^2 - 7k)Q \quad (21)$$

A rearrangement of the terms yields

$$6N - 2(3k^2 + k - 1)S + k^2(3k+7)^2 - 72k - 7 \leq (kQ + S - 3k^2 - 7k)^2 \quad (22)$$

If this relation is fulfilled for a certain Q, it will certainly be fulfilled for $Q' > Q$, since the right-hand side increases with Q while the left-hand side is unchanged under the given circumstances. This proves lemma 1.

Figure 7 illustrates the lemma. In these examples, $B(N;S) = C_{22}H_{12}$, an extremal benzenoid (anthanthrene).

Assume the transformation of formulas $(N^O; S^O) \rightarrow (N^O + Q - 6; S^O + Q - 6)$, which pertains to the circular benzenoids $O(N^O;S^O)$ and circular mono-Q-benzenoids $O_Q(n^O;s^O)$. The formula of O_Q is given by eq 13 in terms of $S = S^O$, which originates from the initial circular benzenoid formula. Consider the formula which corresponds to circum-O_Q and designate it $(n_1^O; s_1^O)$. Then

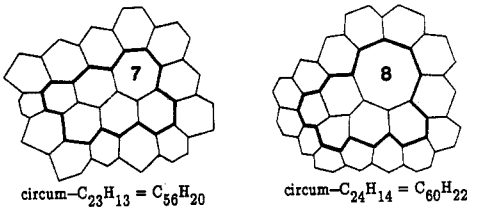

Figure 7. Two nonextremal mono-Q-fusenes (which are mono-Q-benzenoids). Inscribed numerals indicate the size of the Q-gon. The smaller systems, indicated by the heavy-line boundaries, are extremal.

$$(n_1^O; s_1^O) = (3S + 4Q - 18 + 2\lfloor {}^1/_{12}(S^2 - 6S) \rfloor; S + 2Q - 6) \quad (23)$$

Here we allow for all $S \geq 6$, including $S = 7$, which corresponds to the degenerate (non-benzenoid) system C_7H_7 (see Figure 6).

Theorem 1. Circumscribed O_Q, circum-O_Q, is an extremal mono-Q-benzenoid if and only if $Q = 7$ or $O_Q = C_8H_8$ ($Q = 8$, $h = 0$).

Proof. Apply eq 14 to $(n_1^O; s_1^O)$ from eq 23. It should be shown that

$$\lceil (12S + 12Q - 63 + 12\lfloor {}^1/_{12}(S^2 - 6S) \rfloor)^{1/2} \rceil = S + Q - 3 \quad (24)$$

in order to prove that (circum-O_Q)$(n_1^O;s_1^O)$ is extremal. If an integer A satisfies (a) $A < x + 1$ and (b) $A \geq x$, then $A = \lceil x \rceil$. On the other hand, $x - 1 < \lfloor x \rfloor \leq x$.

Condition a, viz.,

$$(12S + 12Q - 63 + 12\lfloor {}^1/_{12}(S^2 - 6S) \rfloor)^{1/2} + 1 > S + Q - 3 \quad (25)$$

yields after some elementary manipulations

$$12\lfloor {}^1/_{12}(S^2 - 6S) \rfloor > S^2 - 20S + Q(2S + Q - 20) + 79 \quad (26)$$

A further rearrangement gives

$$\lfloor {}^1/_{12}(S^2 - 6S) \rfloor > {}^1/_{12}(S^2 - 6S) - 1 + {}^1/_{12}(Q-7)(2S + Q - 13) \quad (27)$$

Case $Q = 7$. In this case eq 27 gives

$$\lfloor {}^1/_{12}(S^2 - 6S) \rfloor > {}^1/_{12}(S^2 - 6S) - 1 \quad (28)$$

which is always satisfied. But it is also necessary to verify condition b, viz. (for $Q = 7$),

$$(12S + 21 + 12\lfloor {}^1/_{12}(S^2 - 6S) \rfloor)^{1/2} \leq S + 4 \quad (29)$$

Herefrom one obtains

$$\lfloor {}^1/_{12}(S^2 - 6S) \rfloor \leq S^2 - 4S - 5 \quad (30)$$

and by a further rearrangement:

$$\lfloor {}^1/_{12}(S^2 - 6S) \rfloor \leq {}^1/_{12}(S^2 - 6S) + {}^1/_{12}(2S - 5) \quad (31)$$

This relation is valid when

$$2S - 5 \geq 0 \quad (32)$$

i.e. when $S \geq 3$, and therefore always in the range of interest for S, viz., $S \geq 6$. This completes the proof of the first part (for $Q = 7$) of theorem 1.

The inclusion of $S = 7$ catches up the special extremal monoheptabenzene $C_{31}H_{15}$. It is depicted in Figure 8 together with an ordinary example, incidentally for $S = 11$.

Case $Q > 7$. Turning back to eq 27, it is ascertained that it can only be satisfied if (but not necessarily if)

$$^1/_{12}(Q-7)(2S+Q-13) < 1 \quad (33)$$

or (as $Q \neq 7$)

$$S < 6(Q-7)^{-1} + {}^1/_2(13-Q) \quad (34)$$

Since $S \geq 6$, it is found that $Q > 8$ is impossible. Only for $Q = 8$ one finds $S < 8.5$, which leaves the possibilities $S = 6, 7, 8$. An inspection of the original criterion, as manifested in eq 19, reveals that only $S = 6$ out of these three values fulfills the requirement. This completes the proof of theorem 1. It is unnecessary to consider condition b; it must certainly be satisfied for $Q = 8$, $S = 6$ by virtue of our direct inspection of eq 19. This case corresponds to (in consistency with theorem 1) $C_{32}H_{16}$ octacirculene (Figure 1), which represents an extremal monooctabenzenoid.

Assume as in theorem 1 the transformation $(N^O; S^O) \rightarrow (N^O + Q - 6; S^O + Q - 6)$. Consider now the formula which corresponds to k-fold circumscribed O_Q, viz., (k-circum-O_Q)-$(n_k{}^O; s_k{}^O)$. Then one finds the following generalization of eq 23 (which pertains to $k = 1$).

$$(n_k{}^O; s_k{}^O) = ((2k+1)(S-6) + (k+1)^2Q + 2\lfloor {}^1/_{12}(S^2-6S)\rfloor; S + (k+1)Q - 6) \quad (35)$$

Theorem 2. In the set of k-fold circumscribed O_Q (k-circum-O_Q) for $k > 1$, twofold circumscribed C_7H_7 ($Q = 7$, $h = 0$) is the only extremal system.

Proof. Consider first the case of $Q = 7$. Criterion 14, when applied to $(n_k{}^O; s_k{}^O)$ from eq 35 with this Q value, yields

$$\lceil (12kS + 3(14k^2 - 10k + 3) + 12\lfloor {}^1/_{12}(S^2-6S)\rfloor)^{1/2} \rceil = S + 7k + 3 \quad (36)$$

as the condition for the system to be extremal. Following the same approach as in the proof of theorem 1, condition a therein gives

$$\lfloor {}^1/_{12}(S^2-6S)\rfloor > {}^1/_{12}(S^2-6S) - 1 + {}^1/_{12}(k-1)(2S+7k-19) \quad (37)$$

A necessary (but not sufficient) condition for 37 to be valid is

$$^1/_{12}(k-1)(2S+7k-19) < 1 \quad (38)$$

The case of $k = 1$ pertains to theorem 1. Now the case of $k \neq 1$ is of interest, and in that case one obtains

$$S < 6(k-1)^{-1} + {}^1/_2(19-7k) \quad (39)$$

A simple analysis shows that $k > 2$ is impossible, and for $k = 2$, $S < 8.5$. That leaves the possibilities $S = 6, 7, 8$. An inspection of condition 36 reveals that only $S = 6$ fulfills the requirement. It is unnecessary to consider condition b specified under theorem 1; it must certainly be satisfied for $k = 2$, $S = 6$ by virtue of the direct inspection of eq 36. The first part of theorem 2 is proved, as far as the case of $Q = 7$ is concerned. In order to employ lemma 1, it is necessary to investigate whether $k = 2$, $S = 6$ gives an extremal monooctabenzenoid. It would be the 2-fold circumscribed C_8H_8 octagon, viz., $C_{72}H_{24}$ in consistency with eq 35. An inspection of the fundamental criterion 14 shows that $C_{72}H_{24}$ is a nonextremal monooctafusene. Then, by lemma 1, there is no extremal k-circum-O_Q for $k > 1$ and $Q \geq 8$. This completes the proof of theorem 2.

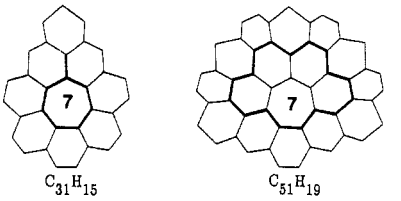

Figure 8. Two extremal monoheptabenzenoids. Inscribed numerals indicate the heptagons. The heavy lines suggest the generation of these systems (see the text).

Assume the transformation $B(N;S) \rightarrow B'$ as in lemma 1 but restricted to noncircular fusenes B and noncircular mono-Q-fusenes B′. Here B and B′ may be extremal or nonextremal. For a circular benzenoid with the same S value as in B, viz., $O(N^O;S)$, the number of hexagons is $H^O = H_{max}$. Since $N^O = 2H^O + S - 2$ and $N = 2H + S - 2$, one has $N < N^O$, and N is at least two units less than N^O. Hence, according to eq 13,

$$N = S + 2\lfloor {}^1/_{12}(S^2-6S)\rfloor - 2\delta \quad (40)$$

where $\delta \geq 1$ (actually $\delta = 2, 4, 6, \ldots$). Consider the formula of k-circum-B′, for example, $(n_k'; s_k')$, for which one finds (similarly to eq 35)

$$(n_k'; s_k') = ((2k+1)(S-6) + (k+1)^2Q + 2\lfloor {}^1/_{12}(S^2-6S)\rfloor - 2\delta; S + (k+1)Q - 6) \quad (41)$$

Theorem 3. The system $M_Q(n_k';s_k')$ is a nonextremal mono-Q-fusene.

Proof. Suppose that circum-B′ was extremal for $Q = 7$. Then, using this Q value together with $k = 1$ in 41, one would have according to criterion 14

$$\lceil (12S + 21 + 12\lfloor {}^1/_{12}(S^2-6S)\rfloor - 12\delta)^{1/2} \rceil = S + 4 \quad (42)$$

Following the same approach as that in the proof of theorem 1, condition a therein leads to

$$\lfloor {}^1/_{12}(S^2-6S)\rfloor > {}^1/_{12}(S^2-6S) + \delta - 1 \quad (43)$$

Since $\delta \geq 1$, this means $\lfloor x \rfloor > x$, a contradiction. Hence, theorem 3 is proved for $k = 1$, $Q = 7$. In other words, a circumscribed noncircular monoheptafusene is nonextremal. But a nonextremal monoheptafusene is also noncircular. Therefore, by a further circumscribing, one arrives at a nonextremal system again. Thus, by complete induction, it is inferred that the theorem is true for any $k \geq 1$. Next, it is ascertained by lemma 1 that also the formula of k-circum-B′ for $k \geq 1$, $Q \geq 8$ corresponds to a nonextremal mono-Q-fusene. That completes the proof of theorem 3.

Ideally speaking, one should have the ambition to account for all the kinds of forms of extremal mono-Q-benzenoids. Actually, we believe that they are already accounted for

through the above arguments, but this is not rigorously proved. We shall presently put forward a conjecture to this effect.

Refer to an extremal (circular) mono-Q-benzenoid with the Q-gon at its perimeter as "common". Otherwise it is "uncommon".

Conjecture 1. (i) An extremal monoheptabenzenoid (Q = 7) is uncommon if and only if it is a circumscribed circular monoheptabenzenoid or the isomer of $C_{31}H_{15}$ depicted in Figure 8 (corresponding formally to circumscribing of the degenerate system C_8H_8). (ii) Octacirculene is the only uncommon extremal monooctabenzenoid (Q = 8). (iii) No uncommon extremal mono-Q-benzenoid exists for $Q > 8$.

Notice that heptacirculene is a circular monoheptabenzenoid, so that circumheptacirculene (the 2-fold circumscribed heptagon) is included under point i in the conjecture. Circumheptacirculene is believed to be the only uncommon circular mono-Q-benzenoid. Octacirculene mentioned under point ii is not circular! Perhaps a misleading designation, but octacirculene has not the maximum number of hexagons in relation to its perimeter length. Similarly, any [Q]circulene for $Q > 8$ is noncircular. In the following, some arguments are offered in support of conjecture 1. The conjecture would be proved if one could demonstrate that the form of any uncommon extremal mono-Q-benzenoid, apart from $C_{31}H_{15}$ (Q = 7), is a circumscribed (smaller) mono-Q-benzenoid. These systems are completely accounted for in theorems 1–3.

Very much is known about the forms of extremal benzenoids,[23–30] which have been identified with the members of constant-isomer series.[6,27,29–34] These systems have no cove or fjord or, more generally, no latent row of hexagons.[27,28] Furthermore, they never possess a hexagon in L_1 among the addition modes when disregarding naphthalene. Extremal benzenoids with more than nine hexagons (disregarding the "edge effects" for the smallest systems again) possess each at most one hexagon in the mode P_2.[28] All these features can be adapted to extremal mono-Q-benzenoids.

Now it seems crucial to demonstrate that an uncommon extremal mono-Q-benzenoid with one P_2-mode hexagon is impossible, apart from $C_{31}H_{15}$ (Q = 7). Suppose that $M_Q(n;s)$ is such a system. The Q-gon is surrounded by hexagons, so it is fair to assume that the system M_Q is a circumscribed mono-Q-benzenoid, say $M_Q(n';s')$, if the P_2-mode hexagon is deleted. The addition of P_2 gives an increment $+C_3H$; hence

$$(n; s) = (n' + 3; s' + 1) \tag{44}$$

Assume that $M_Q'(n';s')$ = circum-$M_Q''(n'';s'')$. Then, according to eq 3,

$$(n'; s') = (n'' + 2s'' + Q; s'' + Q) \tag{45}$$

which was inserted into eq 44 with the result

$$(n; s) = (n'' + 2s'' + Q + 3; s'' + Q + 1) \tag{46}$$

When rewritten in the form

$$(n; s) = ((n'' + 1) + 2(s'' + 1) + Q; (s'' + 1) + Q) \tag{47}$$

it is seen that there will exist an isomer of M_Q, for example, $M_Q^{\dagger}(n;s)$ as circum-$M_Q^*(n^*;s^*)$, where

$$(n^*; s^*) = (n'' + 1; s'' + 1) \tag{48}$$

provided that the invariants of (n^*; s^*) fall within the range which is allowed for the mono-Q-benzenoids. The formula (n''; s'') is compatible with a mono-Q-benzenoid, while the formula (n^*; s^*) is seen to be shifted one place to the left in the table of formulas in our representation (cf. Table 1). It will certainly correspond to a mono-Q-benzenoid M_Q^* unless (n''; s'') is a formula for a catacondensed mono-Q-benzenoid. Suppose this is not the case. Then it is clear that M_Q^* is nonextremal; it has one internal vertex less than M_Q'' and the same number of hexagons. Consequently, $M_Q^{\dagger}$ = circum-M_Q^* is nonextremal by theorem 3. But, then, all the isomers of $M_Q^{\dagger}$, which have the formula (n; s), are nonextremal, and therefore also the original system M_Q.

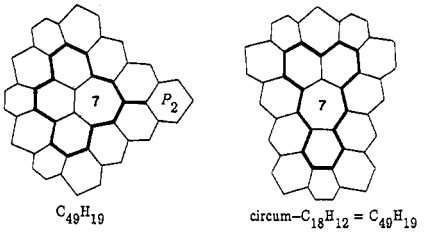

Figure 9. Two nonextremal monoheptabenzenoid isomers of $C_{49}H_{19}$. The P_2-mode hexagon is indicated.

In order to complete this demonstration, one should prove that $M_Q(n;s)$ is nonextremal even if $M_Q''(n'';s'')$ is catacondensed. Then, there is no mono-Q-benzenoid (or mono-Q-fusene) corresponding to (n^*; s^*). Nevertheless,

$$(n; s) = (n^* + 2s^* + Q; s^* + Q) \tag{49}$$

follows the formalism for circumscribing from eq 3. Since M_Q'' is catacondensed, it has the formula

$$(n''; s'') = (Q + 4t; Q + 2t) \tag{50}$$

where t = 0, 1, 2, ... It follows that

$$(n^*; s^*) = (Q + 4t + 1; Q + 2t + 1) \tag{51}$$

and on inserting from eq 51 into eq 49,

$$(n; s) = (4Q + 8t + 3; 2Q + 2t + 1) \tag{52}$$

From eq 14 one obtains

$$\lceil (12Q + 36t + 21)^{1/2} \rceil = Q + 2t + 4 \tag{53}$$

as the criterion for $M_Q(n;s)$ to be extremal. Condition a under the proof of theorem 1 yields after some elementary manipulations

$$Q < 3 - 2t + (12t + 21)^{1/2} \tag{54}$$

A simple analysis of this condition shows that it is never satisfied for $t > 0$ since $Q \geq 7$. Only t = 0, $Q < 7.6$ leaves the possibility for Q = 7. But, this case just gives the exceptional extremal monoheptabenzenoid $C_{31}H_{15}$ of Figure 8.

An illustrative example is furnished by Figure 9. Here M_Q = $C_{49}H_{19}$, M_Q' = $C_{46}H_{18}$, M_Q'' = $C_{17}H_{11}$, M_Q^* = $C_{18}H_{12}$, and $M_Q^{\dagger}$ = $C_{49}H_{19}$ as an isomer of M_Q.

Enumeration of the Circular Systems. The enumeration of the common circular mono-Q-benzenoids is equivalent to the counting of asterisks in Figure 6. Similar problems are the enumeration of circular coronoids[35] and of circular benzenoids perforated by coronene holes.[36] For the sake of brevity we give no details of the derivations here. Table 4 shows the explicit formulas for the numbers in question, I_k, and the corresponding generating functions, $I(x)$. Numerical values are displayed in Table 5.

Enumeration of the Extremal Systems. The counting of asterisks (see above) can be extended to the enumeration of

Table 4. Mathematical Solutions for the Numbers of Nonisomorphic Common Circular Mono-Q-Benzenoids ($Q \geq 7$)[a]

ϵ	I_k	$I(x)$
0	$1 + \lfloor k/2 \rfloor$	$(1-x)^{-1}(1-x^2)^{-1}$
1	$3k + 1$	$(1+2x)(1-x)^{-2}$
2	$k + 1 + \lceil k/2 \rceil$	$(1+2x)(1-x)^{-1}(1-x^2)^{-1}$
3	$k + 1$	$(1-x)^{-2}$
4	$k + 2 + \lfloor k/2 \rfloor$	$(2+x)(1-x)^{-1}(1-x^2)^{-1}$
5	$3(k+1)$	$3(1-x)^{-2}$

[a] The degenerate systems $C_{Q+1}H_{Q+1}$ are included.

Table 5. Numbers of Nonisomorphic Common Circular Mono-Q-Benzenoids ($Q \geq 7$)

	ϵ					
k	0	1	2	3	4	5
0	1	(1)[a]	1	1	2	3
1	1	4	3	2	3	6
2	2	7	4	3	5	9
3	2	10	6	4	6	12
4	3	13	7	5	8	15
5	3	16	9	6	9	18
6	4	19	10	7	11	21
7	4	22	12	8	12	24
8	5	25	13	9	14	27
9	5	28	15	10	15	30
10	6	31	16	11	17	33

[a] Degenerate systems $C_{Q+1}H_{Q+1}$.

Table 6. Numbers of Nonisomorphic Extremal Mono-Q-Benzenoids[a]

		Q		
h	n_i	7	8	≥9
0[c]	0	1	1	1
1[c]	0	1	1	1
2[c]	1	1	1	1
3[c]	2	2	2	2
4[c]	3	3	3	3
5	4	9	9	9
6[c]	6	1	1	1
7[c]	7	5←	4	4
8	8	21←	21←	20
9[c]	10	3	3	3
10	11	19←	18	18
11[c]	13	2	2	2
12	14	26←	25	25
13[c]	16	3	3	3
14	17	41←	39	39
15[c]	19	6	6	6
16	20	93←	90	90
17	22	15	15	15
18[c]	24	2	2	2
19	25	47←	46	46
20[c]	27	7	7	7
21	28	180←	175	175
22	30	34	34	34
23[c]	32	4	4	4
24	33	172←	169	169
25	25	30	30	30

[a] Arrows indicate the presence of uncommon systems; superscript c denotes "circular".

common extremal mono-Q-benzenoids, even when they are not circular. For this purpose we exploited a useful collection of the forms of benzenoids isomers.[34] The results are collected in Table 6.

SURVEY OF NUMBERS OF ISOMERS

A gross survey of the numbers of mono-q-benzenoids ($q < 6$) and mono-Q-benzenoids ($Q > 6$) is shown in Table 7. Only some of these numbers have been given before.[6,7,18,37] As

Table 7. Total Numbers of Simply Connected, Geometrically Planar Mono-$q(Q)$-Polyhexes, Mono-$q(Q)$-Benzenoids

	q			Q		
h	3	4	5	7	8	9
0	1	1[a]	1[b]	1[c]	1	1
1	1	1[a]	1[b]	1[c]	1	1
2	3	4[a]	4[b]	5[c]	6	6
3	11	13[a]	15	20[c]	23	26
4	43	57[a]	69	103[c]	126	146
5	191	255	329	526[c]	654	798
6	884	1224	1635	2796[c]	3587	4513
7	4195	5953	8208	14801[c]	19430	25135

[a] Reference 6. [b] Reference 37. [c] Reference 18.

Table 8. Numbers of Catacondensed Mono-$q(Q)$-Benzenoids

	q			Q		
h	3	4	5	7	8	9
0	1	1	1[a]	1[b]	1	1
1	1	1	1[a]	1[b]	1	1
2	2	3	3[a]	4[b]	5	5
3	6	8	9	13[b]	16	18
4	19	29	35	56[b]	72	84
5	70	103	134	231[b]	299	372
6	260	403	545	999[b]	1329	1714
7	1006	1578	2211	4276[b]	5804	7723
8	3926	6326	9085	18393	25525	34778

[a] Reference 37. [b] Reference 18.

expected by and large (and definitely for $h > 2$), the numbers for a given h increase when $q(Q)$ increases.

Similarly, Table 8 is a collection of numbers of catacondensed mono-$q(Q)$-benzenoids, most of them original data. The formulas are $C_{Q+4h}H_{Q+2h}$. Here again the numbers for given h values increase with increasing $q(Q)$, definitely when $h > 2$.

CONCLUSION

A comprehensive treatment of the theory of mono-Q-fusenes ($Q > 6$) is given for the first time. The properties of these systems are largely different from those of mono-q-fusenes ($q < 6$), which have been known better for some time. The latter category contains biphenylenoids ($q = 4$)[6] and fluoranthenoids/fluorenoids ($q = 5$).[7-9] An extensive enumeration of C_nH_s isomers of mono-Q-benzenoids for $Q = 8$ is reported in the present work. Since tetraphenylene is an outstanding member of this class, it is proposed that these systems be referred to as tetraphenylenoids.

Extremal mono-Q-benzenoids were treated in detail and, in particular, their properties with respect to circumscribing. In this respect the differences from extremal mono-q-benzenoids are most pronounced. One finds, for instance, no constant-isomer series among the chemical formulas of extremal mono-Q-benzenoids ($Q > 6$), while this is a characteristic phenomenon for mono-q-benzenoids ($q < 6$).[31-33]

Mono-$q(Q)$-fusenes are divided into mono-$q(Q)$-benzenoids and mono-$q(Q)$-helicenes. The extremal systems belong to the mono-$q(Q)$-benzenoids. The present work contains no specific treatment of the mono-Q-helicenes, which is left for future considerations. An enumeration of catacondensed mono-Q-fusenes for some values of $Q > 6$ would be interesting, parallel to the corresponding problem for $q = 5$, of which a complete mathematical solution recently has been accomplished.[38] The enumeration data from such a solution could, in the next turn, be used to enumerate the catacondensed mono-Q-helicenes specifically.

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