match no. 26 pp. 63-86 1991

ISOMER ENUMERATION OF CATAFUSENES, $C_{4h+2}H_{2h+4}$ BENZENOID AND HELICENIC HYDROCARBONS[1]*

Sven J. CYVIN, Bjørg N. CYVIN
and Jon BRUNVOLL
Division of Physical Chemistry, The University of Trondheim,
N–7034 Trondheim–NTH, Norway
(received: January 1991)

An introduction to the enumeration of catafusenes (certain polyhex systems which have chemical counterparts in $C_{4h+2}H_{2h+4}$ arenes) is given. Explicit mathematical formulas are presented for the numbers of catafusenes belonging to different symmetries.

---

* Dedicated to Professor, Dr.–Ing. Bernhard Schrader on his 60th birthday. The reader is also referred to *Acknowledgements.*

1 Introduction

The enumeration of chemical isomers is a classical problem, especially in organic chemistry.[2] Perhaps best known is the question, which has been asked at least 125 years ago:[3] – How many alkanes with the formula C_nH_{2n+2} can be constructed? Already in this old problem the "topological" isomers were counted, as we today would call an enumeration of nonisomorphic chemical graphs.[4] Within this frame, e.g. Schrader[2] listed 1 isomer each of methane, ethane and propane, 2 butanes and 3 pentanes. Now we know the numbers through $n = 80$; the number of $C_{80}H_{162}$ alkane isomers is:[5]

10 564 476 906 946 675 106 953 415 600 016

When the polycyclic aromatic hydrocarbons (arenes) are considered, Schrader's book[2] (among almost every textbook in organic chemistry) includes 1 isomer of C_6H_6 benzene, 1 of $C_{10}H_8$ naphthalene, but 2 $C_{14}H_{10}$ isomers, viz. anthracene and phenanthrene. This is actually the start of an enumeration of catafusene isomers, the topic of the present paper.

2 Catafusene Systems and Hydrocarbons

2.1 Definitions

The terminology in mathematical chemistry of polyhexes (benzenoids, fusenes, hexagonal systems, hexanimals, etc.) is manifold and partly controversial.[6–8] Therefore it is especially important to define the terms which shall be used presently.

A polyhex system (or briefly polyhex) is a connected geometrical object consisting of congruent regular hexagons, where any two hexagons either share one and only one edge, or they are completely disjoint. A polyhex has a chemical counterpart in a polycyclic hydrocarbon (synthesized or hypothetical) with six–membered (benzenoid) rings exclusively. Such a ring corresponds to what was referred to as a hexagon in the above definition.

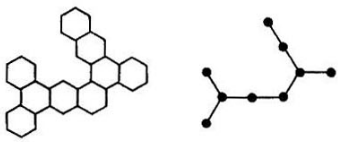
A *catafusene*[9] (system) is a catacondensed, simply connected polyhex. A catacondensed system has no internal vertices; an internal vertex is shared by three hexagons. The simple connectivity implies that there should not be "holes", and therefore coronoids[6,10] (circulenes, coronafusenes, etc.) are excluded.

The chemical formula of a catafusene hydrocarbon is $C_{4h+2}H_{2h+4}$, where h is the number of hexagons.

A catafusene may be either a geometrically planar or a geometrically nonplanar system, and is accordingly referred to as a catacondensed *benzenoid* (system) or a catacondensed *helicenic* system (shortly called helicene), respectively. We shall refer to these classes still shorter as *catabenzenoids* and *catahelicenes*.

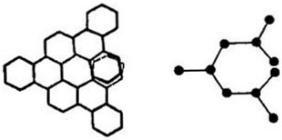
Finally it is distinguished between *unbranched* and *branched* catafusenes both among catabenzenoids and catahelicenes. A branched catafusene has at least one branching hexagon, which is directly connected to three other hexagons.

A polyhex may be represented in terms of hexagons; usually drawn so that two edges of each hexagon are vertical. An alternative representation is the dualist,[11] where each point (black circle) represents a hexagon. Below is a catafusene depicted in these two representations.



2.2 Examples

Polycyclic hydrocarbons (arenes) which correspond to catabenzenoids, both branched and unbranched, are known in copious amounts from organic chemistry.[12] But also a great number of helicenic hydrocarbons (helicenes) have been synthesized, the first of them being hexahelicene or [6]helicene.[13] It was followed by a homologous series corresponding to unbranched catahelicenes up to [14]helicene.[14] Also interesting is a synthesis of $C_{42}H_{24}$, a branched helicene:[15]



It was mentioned that coronoids fall outside the class of catafusenes. A corresponding hydrocarbon among molecules with "holes" and belonging to a class called cycloarenes, is the famous $C_{48}H_{24}$ kekulene;[16] notice that its formula is not compatible with $C_{4h+2}H_{2h+4}$.

Additional examples of catafusenes ($C_{4h+2}H_{2h+4}$), presented in a more systematic way, are found in the following section on symmetry.

3 Symmetry

3.1 Definitions, some Properties, and Notation

Benzene ($h = 1$) is the only catafusene of regular hexagonal symmetry, D_{6h}. Otherwise the catafusenes are distributed among the symmetry groups D_{3h}, C_{3h}, D_{2h}, C_{2h}, C_{2v} and C_s. In this classification the nonplanarity of helicenes is not taken into account; the catahelicene $C_{42}H_{24}$ in Paragraph 2.2, for instance, is classified under C_{2v}. Certain subdivisions of the symmetry groups of interest have been defined.[6] In the present context it is especially important to distinguish between C_{2v}(a) and C_{2v}(b), depending on whether the two-fold symmetry axis cuts edges or passes through vertices, respectively. Otherwise one finds that all trigonal catafusenes are of the first kind,

D_{3h}(i) or C_{3h}(i), characterized by possessing a central hexagon each. A further subdivision places all regular trigonal catafusenes into D_{3h}(ia) inasmuch as all their two–fold symmetry axes cut edges. The dihedral (D_{2h}) and centrosymmetrical (C_{2h}) polyhexes are in general of the first or second kind, depending on whether the number of hexagons is odd or even, respectively. Those of the first kind, identified by D_{2h}(i) and C_{2h}(i), have a central hexagon each; those of the second kind, viz. D_{2h}(ii) and C_{2h}(ii), have a central edge each.

All trigonal (D_{3h} and C_{3h}) catafusenes are branched. Those belonging to D_{2h} are branched except for the single linear chains (polyacenes). Catafusenes belonging to each of the classes C_{2h}, C_{2v}(a), C_{2v}(b) and C_s are either branched or unbranched.

In the following the numbers of nonisomorphic catafusenes of a certain class and having h hexagons are denoted by X_h, where X stands for the following symbols in the different cases.

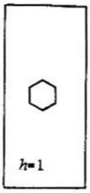
I:	# regular hexagonal (D_{6h}) catafusenes (trivial)
T:	# regular trigonal (D_{3h}) catafusenes
R:	# nonregular trigonal (C_{3h}) catafusenes
D:	# dihedral (D_{2h}) catafusenes
C:	# centrosymmetrical (C_{2h}) catafusenes
$M^{(a)}$:	# mirror–symmetrical catafusenes belonging to C_{2v}(a)
$M^{(b)}$:	# mirror–symmetrical catafusenes belonging to C_{2v}(b)
U:	# unsymmetrical (C_s) catafusenes

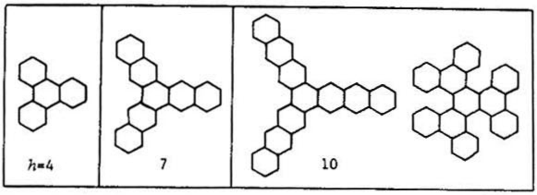
3.2 Examples

Figure 1 shows, in a systematic way, the smallest catabenzenoids of different symmetries, and also hexahelicene under C_{2v}(b), $h = 6$.

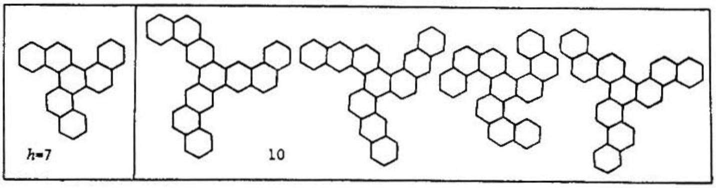
Catahelicenes are most conveniently depicted as dualists. Figure 2 shows the

D_{6h} D_{3h}

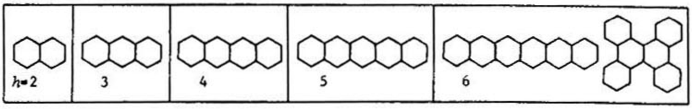




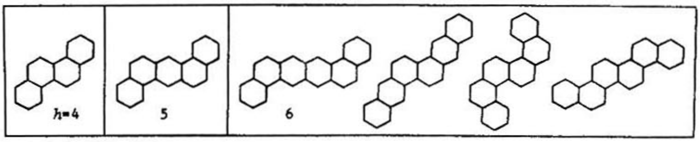
C_{3h}



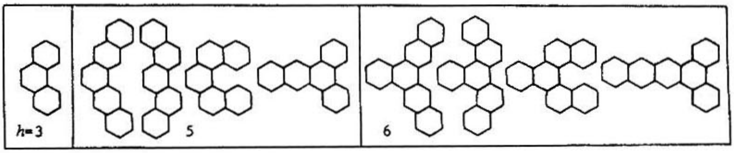
D_{2h}



C_{2h}



C_{2v}(a)



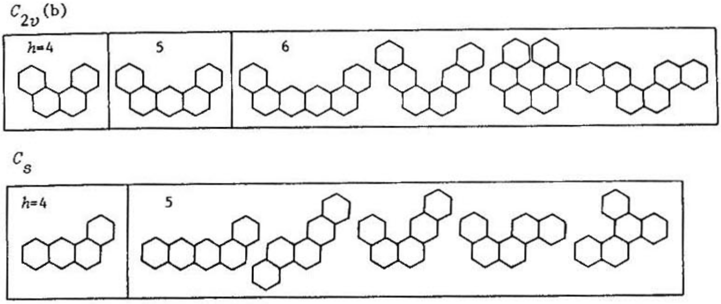
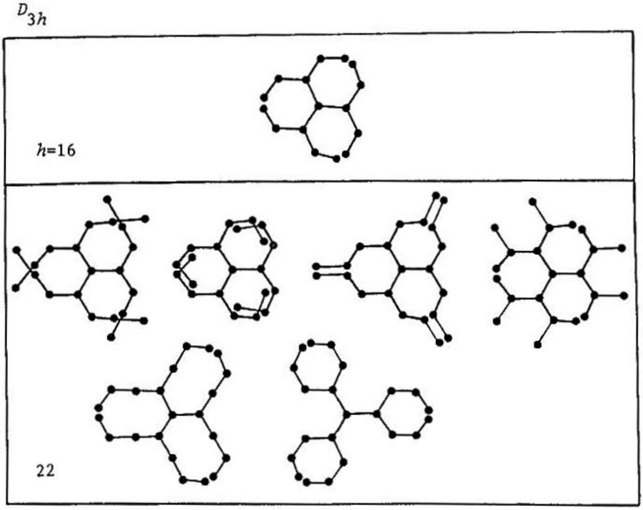
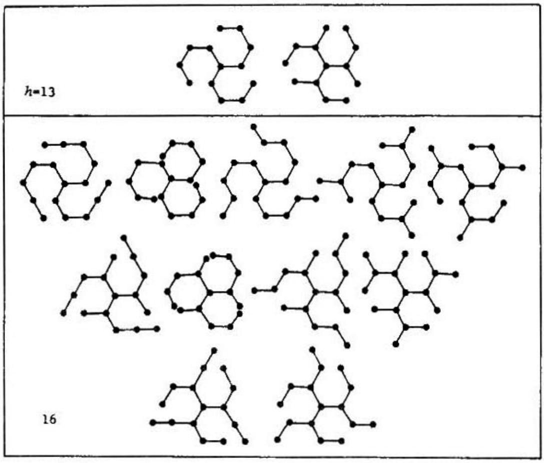


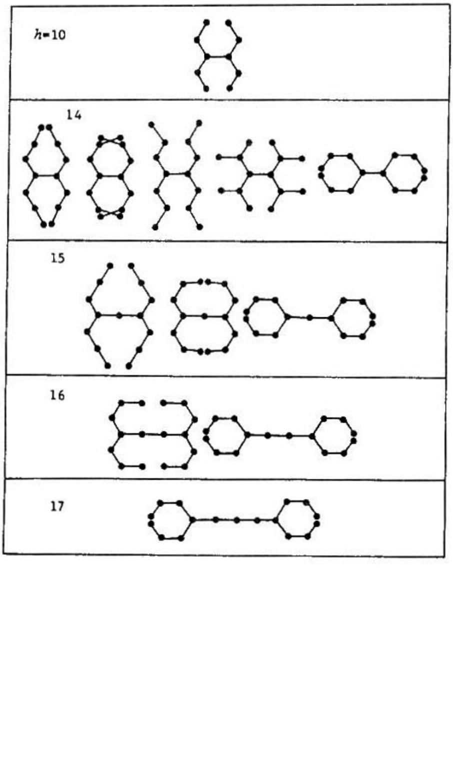
Fig. 1. Forms of the smallest catabenzenoids of different symmetries, including one catahelicene.



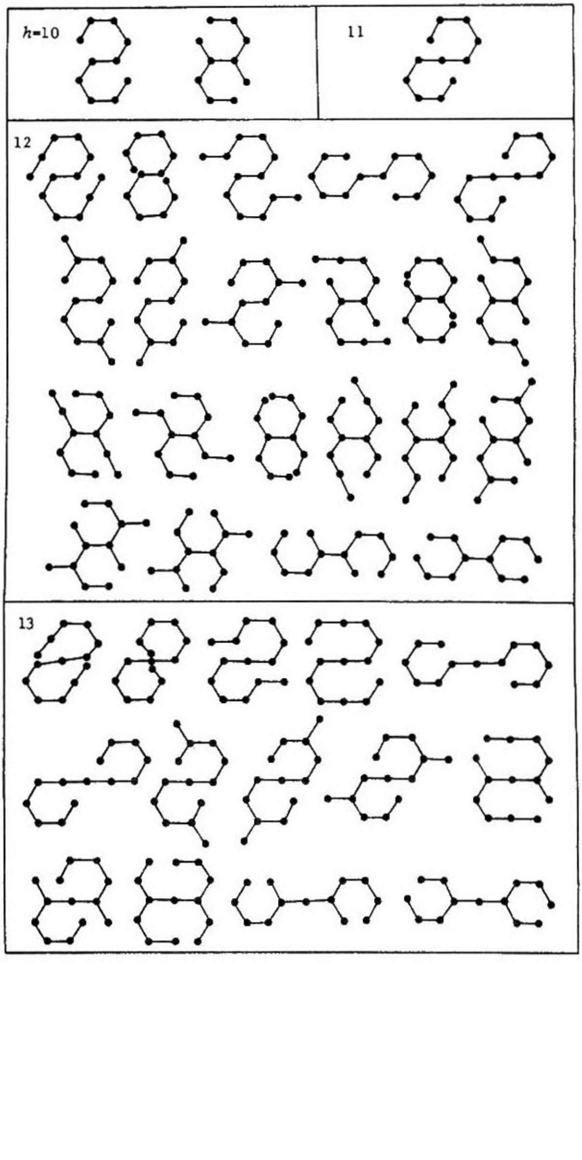
C_{3h}



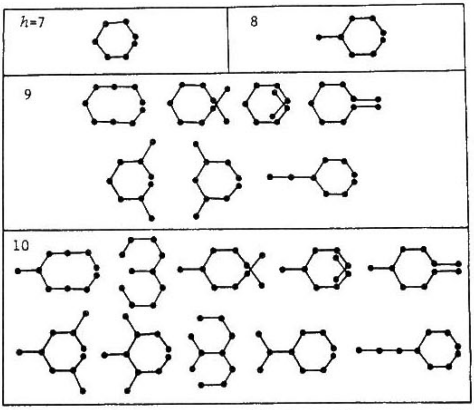
D_{2h}



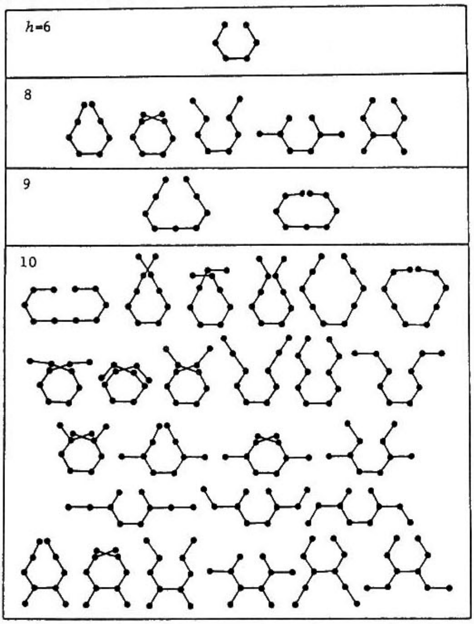
C_{2h}



C_{2v}(a)



C_{2v}(b)



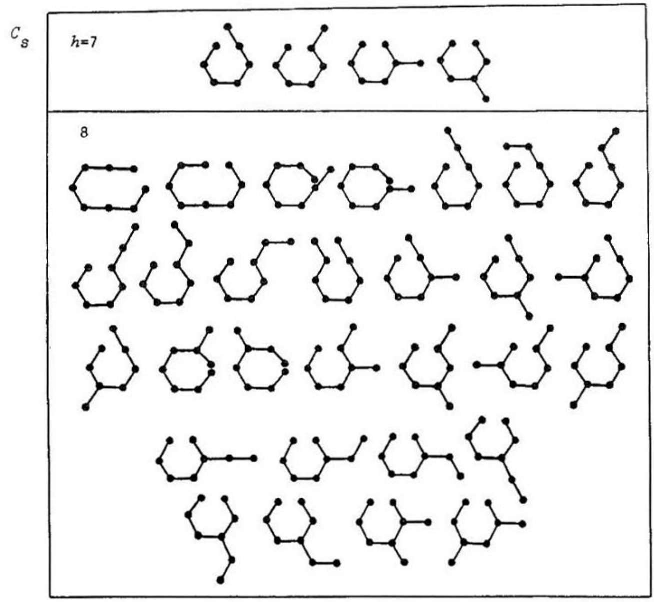


Fig. 2. Forms of the smallest catahelicenes of different symmetries. The dualist representation is employed.

forms of the smallest such systems of different symmetries.

4 Catafusenes Rooted at an Edge

The first task in the analytical enumeration of catafusenes concerns the systems rooted at an edge. It means that a unique "root edge" is distinguished in one of the hexagons. It is not allowed to add any other hexagon incident to the root edge.

Neither is any symmetry operation allowed. Hence, for 2 hexagons for instance, there will be three rooted naphthalenes:

Here the root edge is indicated in bold. Figure 3 shows the forms of the "edge–rooted" catafusenes (as dualists) for 2 and 3 hexagons.

Harary and Read[17] have given a general solution for the numbers of edge–rooted catafusenes in terms of a generating function. Below we present an alternative form of this solution.

$$N_0 = N_1 = 1 \;,\; N_2 = 3 \;,\; N_{x+1} = N_x + \sum_{i=1}^{x-1} N_i N_{x-i} \; (x > 1) \tag{1}$$

Also this recursive algorithm (like the generating function) allows the computation of N_x with arbitrarily large x. Table 1 shows the numerical values up to $x = 20$. The definition $N_0 = 1$ is convenient to make in view of the deductions in the following.

5 Catafusenes Classified According to Symmetry

5.1 *Preliminaries*

The numbers of edge–rooted catafusenes (N_x) give a clue to the enumeration of (unrooted) catafusenes. We have in fact achieved to express the numbers of nonisomorphic catafusenes belonging to any of the symmetries of interest explicitly in terms of the N_x numbers.

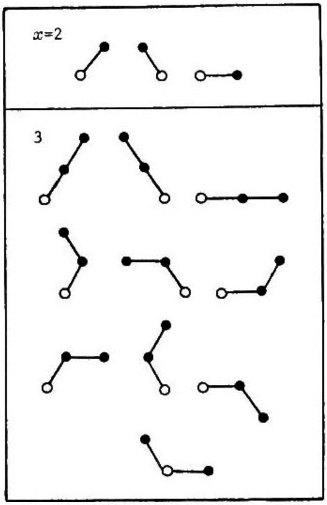


Fig. 3. Forms of the edge–rooted catafusenes with 2 and 3 hexagons. The dualist representation is employed. White circles represent hexagons containing root edges.

Table 1. Numerical values of N_x, the numbers of edge–rooted catafusenes with x hexagons. Trivial value: $N_0 = 1$.

x	N_x	x	N_x
1	1	11	751 236
2	3	12	3 328 218
3	10	13	14 878 455
4	36	14	67 030 785
5	137	15	304 036 170
6	543	16	1 387 247 580
7	2 219	17	6 363 044 315
8	9 285	18	29 323 149 825
9	39 587	19	135 700 543 190
10	171 369	20	630 375 241 380

5.2 Symmetry D_{6h}

$$I_h = \lfloor 1/h \rfloor \quad (2)$$

This is the trivial case. Here and in the following we make use of the "floor" function: $\lfloor a \rfloor$ is the largest integer smaller than or equal to a.

5.3 Symmetry D_{3h}

$$T_1 = T_2 = T_3 = 0 \ , \quad T_h = (\lfloor (h-1)/3 \rfloor - \lfloor (h-2)/3 \rfloor) \sum_{i=0}^{\lfloor (h-4)/6 \rfloor} N_i \quad (h > 3) \quad (3)$$

5.4 Symmetry C_{3h}

$$R_1 = R_2 = R_3 = 0$$

$$R_h = \tfrac{1}{2}(\lfloor (h-1)/3 \rfloor - \lfloor (h-2)/3 \rfloor)\Big[N_{\lfloor (h-1)/3 \rfloor} - \sum_{i=0}^{\lfloor (h-4)/6 \rfloor} N_i\Big] \quad (h > 3) \quad (4)$$

5.5 Symmetry D_{2h}

$$D_1 = 0 \ , \quad D_h = \sum_{i=0}^{\lfloor (h-2)/4 \rfloor} N_i \quad (h > 1) \quad (5)$$

5.6 Symmetries C_{2h} and C_{2v}(b)

$$C_1 = M_1^{(b)} = 0 \ , \quad C_h = M_h^{(b)} = \tfrac{1}{2} N_{\lfloor h/2 \rfloor} - \tfrac{1}{2} \sum_{i=0}^{\lfloor (h-2)/4 \rfloor} N_i \quad (h > 1) \quad (6)$$

5.7 Symmetry C_{2v}(a)

$$M_1^{(a)} = M_2^{(a)} = 0 \ , \ M_3^{(a)} = 1$$

$$M_h^{(a)} = \tfrac{1}{2}\,[2-(-1)^h]\,N_{\lfloor h/2\rfloor} - \tfrac{1}{2}\sum_{i=0}^{\lfloor (h-2)/4\rfloor} N_i \tag{7}$$
$$-\,(\lfloor (h-1)/3\rfloor - \lfloor (h-2)/3\rfloor)\sum_{i=0}^{\lfloor (h-4)/6\rfloor} N_i \quad (h>3)$$

5.8 Symmetry C_s

$$U_1 = U_2 = U_3 = 0 \ , \ U_4 = 1 \ , \ U_5 = 5$$

$$U_h = \tfrac{1}{2}\,N_{h-1} + \tfrac{1}{8}\,[1-(-1)^h]\,N_{\lfloor (h-1)/2\rfloor}\,(3N_{\lfloor (h-1)/2\rfloor}+1)$$

$$-\tfrac{1}{4}\,[5-(-1)^h]\,N_{\lfloor h/2\rfloor} - \tfrac{1}{8}\,[1+(-1)^h]\,N_{\lfloor h/2\rfloor}(N_{\lfloor h/2\rfloor}-1)$$

$$+\tfrac{1}{2}\sum_{i=0}^{\lfloor (h-2)/4\rfloor} N_i + \tfrac{3}{2}\sum_{i=1}^{\lfloor (h/2)-1\rfloor} N_i\,N_{h-i-1} - \tfrac{1}{2}\sum_{i=1}^{\lfloor (h-1)/2\rfloor} N_i\,N_{h-i} \tag{8}$$

$$+\tfrac{1}{6}\,(\lfloor (h-1)/3\rfloor - \lfloor (h-2)/3\rfloor)\,\Big[N_{\lfloor (h-1)/3\rfloor}(N_{\lfloor (h-1)/3\rfloor}{}^2-1)$$

$$+\,3\sum_{i=0}^{\lfloor (h-4)/6\rfloor} N_i\Big]$$

$$+\tfrac{1}{2}\sum_{i=1}^{\lfloor (h-2)/3\rfloor} N_i\Big[(N_i\,N_{h-2i-1} + \sum_{j=i+1}^{h-2\,i-2} N_j\,N_{h-i-j-1})\Big] \quad (h>5)$$

5.9 Interrelations

There are many interrelations between the quantities considered above. Some of them are specified in the following.

$$T_h = (\lfloor (h-1)/3 \rfloor - \lfloor (h-2)/3 \rfloor)\, D_{\lfloor (2h-2)/3 \rfloor} \quad (h > 1) \tag{9}$$

$$R_h = \tfrac{1}{2}(\lfloor (h-1)/3 \rfloor - \lfloor (h-2)/3 \rfloor)(N_{\lfloor (h-1)/3 \rfloor} - D_{\lfloor (2h-2)/3 \rfloor})$$

$$= (\lfloor (h-1)/3 \rfloor - \lfloor (h-2)/3 \rfloor) C_{\lfloor (2h-2)/3 \rfloor} \quad (h > 1) \tag{10}$$

$$C_h = M_h^{(\mathrm{b})} = \tfrac{1}{2}(N_{\lfloor h/2 \rfloor} - D_h) \quad (h > 1) \tag{11}$$

$$M_h^{(\mathrm{a})} = \tfrac{1}{2}[2 - (-1)^h] N_{\lfloor h/2 \rfloor} - \tfrac{1}{2} D_h - T_h$$

$$= \tfrac{1}{2}[1 - (-1)^h] N_{\lfloor h/2 \rfloor} + C_h - T_h \quad (h > 1) \tag{12}$$

$$T_h + D_h + M_h^{(\mathrm{a})} + M_h^{(\mathrm{b})} = \tfrac{1}{2}[3 - (-1)^h]\, N_{\lfloor h/2 \rfloor} \quad (h > 1) \tag{13}$$

5.10 Numerical Values

The formulas reported above were used to compute the numbers of interest. Table 2 gives a listing of the results up to $h = 20$. The totals are consistent with the generating function denoted by $H(x)$ from the work of Harary and Read.[17] Furthermore, the sums of numbers according to Eq. (13) are consistent with the generating function $W(x)$ from the same work.[17]

Table 2. Numbers of catafusenes (catabenzenoids + catahelicenes), classified according to symmetry.

h	D_{6h}	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}(a)	C_{2v}(b)	C_s	Total
1	1	0	0	0	0	0	0	0	1
2	0	0	0	1	0	0	0	0	1
3	0	0	0	1	0	1	0	0	2
4	0	1	0	1	1	0	1	1	5
5	0	0	0	1	1	4	1	5	12
6	0	0	0	2	4	4	4	23	37
7	0	1	1	2	4	13	4	98	123
8	0	0	0	2	17	17	17	393	446
9	0	0	0	2	17	53	17	1600	1689
10	0	2	4	5	66	64	66	6486	6693
11	0	0	0	5	66	203	66	26694	27034
12	0	0	0	5	269	269	269	110818	111630
13	0	2	17	5	269	810	269	465890	467262
14	0	0	0	15	1102	1102	1102	1978032	1981353
15	0	0	0	15	1102	3321	1102	8481860	8487400
16	0	5	66	15	4635	4630	4635	36681383	36695369
17	0	0	0	15	4635	13920	4635	159894915	159918120
18	0	0	0	51	19768	19768	19768	701898184	701957539
19	0	5	269	51	19768	59350	19768	3100972840	3101072051
20	0	0	0	51	85659	85659	85659	13779678410	13779935438

6 Branched and Unbranched Catafusenes

6.1 Unbranched Catafusenes

The numbers of unbranched catafusenes, classified according to symmetry, were derived by Balaban and Harary[11] using combinatorial methods. Powers of 3 are the essential ingredients of their explicit mathematical formulas. The numbers of nonisomorphic catafusenes of a certain class and having h hexagons are denoted by x_h, where x stands for the following symbols in the different cases.

a:	# acenes (linear); D_{2h} for $h > 1$, D_{6h} for $h = 1$ (benzene)
c:	# centrosymmetrical (C_{2h}) systems (unbranched catafusenes)
$m^{(a)}$:	# mirror–symmetrical systems belonging to C_{2v}(a)
$m^{(b)}$:	# mirror–symmetrical systems belonging to C_{2v}(b)
u:	# unsymmetrical (C_s) systems

The explicit formulas are given in the following. Most of them are only modified forms[8,18,19] of the original solution;[11] only the subdivision for the types C_{2v}(a) and C_{2v}(b) is new.

Symmetries D_{6h} and D_{2h}:

$$a_h = 1 \tag{14}$$

Symmetries C_{2h} and C_{2v}(b):

$$c_1 = m_1^{(b)} = 0 \ , \quad c_h = m_h^{(b)} = \tfrac{1}{2}\left(3^{\lfloor (h/2)-1 \rfloor} - 1\right) \quad (h > 1) \tag{15}$$

Symmetry C_{2v}(a):

$$m_1^{(a)} = m_2^{(a)} = 0 \ , \quad m_h^{(a)} = \tfrac{1}{2}\left[1-(-1)^h\right] 3^{\lfloor (h-3)/2 \rfloor} \quad (h > 2) \tag{16}$$

Symmetry C_s:

$$u_1 = 0 \ , \quad u_h = \tfrac{1}{4}(3^{h-2}+1) - \tfrac{1}{4}\left[3-(-1)^h\right] 3^{\lfloor (h/2)-1 \rfloor} \quad (h > 1) \tag{17}$$

Numerical values of the numbers of unbranched catafusenes have been listed[8] up to $h = 20$. For these systems also the separate numbers for the catabenzenoids and catahelicenes are available.[8,19] A corresponding analysis for the branched catafusenes is virtually an original contribution of the present work. This issue is treated in the next paragraph.

6.2 Branched Catafusenes

The numbers of branched catafusenes within the classes under consideration are now obtained simply by subtractions. There are no such systems for the D_{6h} symmetry. Otherwise we find the numbers as specified in the following.

D_{3h}: T_h; $\quad C_{3h}$: R_h; $\quad D_{2h}$: $D_h - 1$;

C_{2h}: $C_h - c_h$; $\quad C_{2v}$(a): $M_h^{(a)} - m_h^{(a)}$;

C_{2v}(b): $M_h^{(b)} - m_h^{(b)}$; $\quad C_s$: $U_h - u_h$

In Table 3 the numerical values of the numbers of branched catafusenes are listed (arbitrarily) up to $h = 20$. Herein the specific numbers for the different symmetries are displayed for the first time.

Table 3. Numbers of branched catafusenes (catabenzenoids + catahelicenes), classified according to symmetry.

h	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}(a)	C_{2v}(b)	C_s	Total
4	1	0	0	0	0	0	0	1
5	0	0	0	0	1	0	1	2
6	0	0	1	0	4	0	7	12
7	1	1	1	0	4	0	46	53
8	0	0	1	4	17	4	224	250
9	0	0	1	4	26	4	1080	1115
10	2	4	4	26	64	26	4886	5012
11	0	0	4	26	122	26	21854	22032
12	0	0	4	148	269	148	96177	96746
13	2	17	4	148	567	148	421846	422732
14	0	0	14	738	1102	738	1845536	1848128
15	0	0	14	738	2592	738	8084008	8088090
16	5	66	14	3542	4630	3542	35486734	35498533
17	0	0	14	3542	11733	3542	156309875	156328706
18	0	0	50	16488	19768	16488	691139784	691192578
19	5	269	50	16488	52789	16488	3068694360	3068780449
20	0	0	50	75818	85659	75818	13682833129	13683070474

7 Branched Catabenzenoids and Catahelicenes

7.1 Branched Catabenzenoids

For the numbers of catabenzenoids (without helicenes) of the different classes no exact mathematical solutions are available. But extensive enumerations by computers have been executed in such cases. In Table 4 the numbers of branched catabenzenoids are listed up to $h = 15$. Most of these data are documented in a recent review.[8] They are taken from different sources.[8,18,20–24] The splitting into the (a) and (b) types for the C_{2v} systems is an original contribution.

7.2 Branched Catahelicenes

Numbers of catahelicenes of the classes under consideration are now obtained, up to $h = 15$, simply by subtractions of the numbers of catabenzenoids from those of the catafusenes in total. Here we are all the time speaking about the branched systems exclusively. It should be clear that the results (cf. Table 5) were obtained by a combination of a mathematical analysis and computer programming.

The numbers in Table 5 are seen to be consistent with the depictions of Fig. 2, where the branched systems easily are recognized.

Acknowledgements

Professor, Dr.–Ing. Bernhard Schrader made one of us (SJC) aware of the journal MATCH. This had great consequences for the direction of our research.

This manuscript is written by T^3 [25], a system which Schrader praised long before we started to use it.

Financial support to BNC from the Norwegian Research Council for Science and the Humanities is gratefully acknowledged.

Table 4. Numbers of branched catabenzenoids, classified according to symmetry.

h	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}(a)	C_{2v}(b)	C_s	Total
4	1	0	0	0	0	0	0	1
5	0	0	0	0	1	0	1	2
6	0	0	1	0	4	0	7	12
7	1	1	1	0	4	0	44	51
8	0	0	1	4	16	2	206	229
9	0	0	1	4	23	4	937	969
10	2	4	3	25	54	13	3997	4098
11	0	0	4	26	97	21	16719	16867
12	0	0	4	132	203	66	68520	68925
13	2	15	4	140	400	107	278239	278907
14	0	0	9	620	735	306	1121632	1123302
15	0	0	11	658	1628	468	4504875	4507640

Table 5. Numbers of branched catahelicenes, classified according to symmetry*.

h	C_{3h}	D_{2h}	C_{2h}	C_{2v}(a)	C_{2v}(b)	C_s	Total
7	0	0	0	0	0	2	2
8	0	0	0	1	2	18	21
9	0	0	0	3	0	143	146
10	0	1	1	10	13	889	914
11	0	0	0	25	5	5135	5165
12	0	0	16	66	82	27657	27821
13	2	0	8	167	41	143607	143825
14	0	5	118	367	432	723904	724826
15	0	3	80	964	270	3579133	3580450

* A unique branched catahelicene for D_{3h} occurs at $h = 16$.

References

1 Part 18 of the series "Enumeration and Classification of Benzenoid Hydrocarbons".

2 B. Schrader, *Kurzes Lehrbuch der Organischen Chemie*, Walter de Gruyter, Berlin 1979; 2nd Edit. 1985.

3 E. Cayley, *Ber. Dtsch. Chem. Ges.* **8**, 172 (1875).

4 N. Trinajstić, *Chemical Graph Theory*, Vols. I, II, CRC Press, Boca Raton, Florida 1983.

5 J. V. Knop, W. R. Müller, K. Szymanski and N. Trinajstić, *Computer Generation of Certain Classes of Molecules*, Association of Chemists and Technologists of Croatia, Zagreb 1985.

6 I. Gutman and S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer–Verlag, Berlin 1989.

7 N. Trinajstić, *J. Math. Chem.* **5**, 171 (1990).

8 B. N. Cyvin, J. Brunvoll and S. J. Cyvin, *Advances in the Theory of Benzenoid Hydrocarbons*, Vol. 2 (Ed. I. Gutman), Springer–Verlag, Berlin; *Topics in Current Chemistry*, in press.

9 A. T. Balaban, *Tetrahedron* **25**, 2949 (1969).

10 S. J. Cyvin, J. Brunvoll and B. N. Cyvin, *Theory of Coronoid Hydrocarbons*, Springer–Verlag, Berlin; *Lecture Notes in Chemistry*, **54** (1991).

11 A. T. Balaban and F. Harary, *Tetrahedron*, **24**, 2505 (1968).

12 E. Clar, *Polycyclic Hydrocarbons*, Vol. I, Academic Press, London 1964.

13 M. S. Newman and D. Lednicer, *J. Am. Chem. Soc.* **78**, 4765 (1956).

14 R. H. Martin, *Angew. Chem. Int. Ed. Engl.* **13**, 649 (1974).

15 W. H. Laarhoven and R. J. F. Nivard, *Tetrahedron* **32**, 2445 (1976).

16 H. A. Staab and F. Diederich, *Chem. Ber.* **116**, 3487 (1983).

17 F. Harary and R. C. Read, *Proc. Edinburgh Math. Soc., Ser. II* **17**, 1 (1970).

18 A. T. Balaban, J. Brunvoll, B. N. Cyvin and S. J. Cyvin, *Tetrahedron* **44**, 221 (1988).

19 J. Brunvoll, R. Tošić, M. Kovačević, A. T. Balaban, I. Gutman and S. J. Cyvin, *Rev. Roumaine Chim.* **35**, 85 (1990).

20 W. C. He and W. J. He, *Theor. Chim. Acta* **68**, 301 (1985).

21 W. C. He and W. J. He, *Tetrahedron* **19**, 5291 (1986).

22 J. Brunvoll, B. N. Cyvin and S. J. Cyvin, *J. Chem. Inf. Comput. Sci.* **27**, 171 (1987).

23 W. J. He, W. C. He, Q. X. Wang, J. Brunvoll and S. J. Cyvin, *Z. Naturforsch.* **43a**, 693 (1988).

24 S. J. Cyvin and J. Brunvoll, *Chem. Phys. Letters* **170**, 364 (1990).

25 T^3 Scientific Word Processing System, TCI Software Research, Inc., Las Cruces, New Mexico, USA (1987).