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A PERIODIC TABLE FOR ALL-BENZENOID HYDROCARBONS AND ENUMERATIONS OF SOME POLYHEX ISOMERS

S.J. CYVIN, J. BRUNVOLL and B.N. CYVIN
Division of Physical Chemistry, The University of Trondheim, N-7034 Trondheim-NTH, Norway

Abstract

A polyhex (benzenoid or coronoid) isomer is characterized by the formula C_nH_s, which pertains to the corresponding hydrocarbon. The periodic table for benzenoid hydrocarbons is revisited, and the construction of it is simplified. All-benzenoids are treated with respect to their isomers. A periodic table for all-benzenoid hydrocarbons is proposed, and an easy construction of it is described. It involves the process of "super-circumscribing", a new concept. Numerical data are given for a number of isomer classes of benzenoids, all-benzenoids and single coronoids. These data represent a substantial amount of supplements to the previously known numbers of different polyhex isomers.

1. Introduction

A polyhex has a chemical counterpart in a polycyclic hydrocarbon (chemically known or unknown), for which the formula C_nH_s can be written. In the enumeration of polyhex isomers, one tries to find the number of nonisomorphic polyhex systems corresponding to a given formula C_nH_s. Usually, the enumeration is restricted to certain classes of polyhexes; in the present work the benzenoids, all-benzenoids and coronoids are considered. The reader is referred to two recent monographs [1,2] for a general background and the definitions adopted here. In addition, some special points are emphasized in the following because it is so important to specify exactly which systems actually are enumerated.

A benzenoid (system) is by definition a planar, simply connected polyhex. The all-benzenoids (also called fully benzenoids) form a subclass of benzenoids. It is implied that the benzenoids may be characterized as polyhexes without holes. A coronoid (system) is a planar, multiply connected polyhex. Hence, the coronoids are polyhexes with holes; such a hole, which is called a corona hole, should by definition have a size of at least two hexagons. The present definitions imply that a benzenoid or coronoid may be either Kekuléan or non-Kekuléan. Furthermore, all helicenic (nonplanar) polyhexes are excluded.

A pioneering work on benzenoid isomers is due to Dias [3,4], who invented the periodic table for benzenoid hydrocarbons [3–6]. His enumerations of benzenoid isomers were preceded by Elk [7]. The enumeration and classification of benzenoids according to their number of internal vertices, as executed by the Düsseldorf–Zagreb group [8,9], is virtually a benzenoid isomer enumeration. This is also the case for the enumeration by Stojmenović et al. [10], who employed the perimeter length as the leading parameter [11] and classified the generated systems according to their numbers of hexagons. Furthermore, the enumeration of catacondensed polyhexes is a special isomer enumeration. Two early works in this area should be mentioned, namely those by Balaban and Harary [12] and by Harary and Read [13]. In both of these works, the helicenic systems are included.

Very recently, the pioneering works on benzenoid isomer generation and enumeration by Dias [3–5,14–16] were supplemented and corrected for several numerical errors [17–19]. A first substantial enumeration of coronoid isomers (beyond the catacondensed systems) has been published [20], as well as the corresponding data for some double and triple coronoids [19].

In the present work, the Dias periodic table is revisited, especially with respect to the construction of it. A special periodic table for all-benzenoid hydrocarbons is proposed and discussed. A substantial amount of new enumeration data, mostly obtained by computer aid, are reported.

2. Periodic table for benzenoid hydrocarbons

The periodic table for benzenoid hydrocarbons is a scheme of the possible formulas C_nH_s, which are compatible with benzenoid systems. The formulas are arranged in a coordinate system (d_s, n_i). Here, d_s denotes the number of tree disconnections with reference to the internal edges of the benzenoid [3,4] and is also called the Dias parameter [17,20]. The symbol n_i is used to denote the number of internal vertices.

Figure 1 shows a mapping of the periodic table under consideration. One should imagine a formula C_nH_s in the place of each dot. The table extends infinitely downwards and to the right. The top row pertains to the catacondensed benzenoids. The staircase-like upper-left boundary was determined [2,17] on the basis of the Harary–Harborth [21] analysis of "extremal animals"; cf. also Gutman [22]. The table considered here is the version with even-number and odd-number carbons taken together [17]; thus, it is a fusion of the two periodic tables given separately in one of the Dias publications [5]. The position of benzene (C_6H_6) is troublesome and has been left out. In the following, it shall also be referred to the present version of the table as the general periodic table (of benzenoid hydrocarbons) because certain subsets of it are going to be treated in the subsequent sections.

The general periodic table of benzenoid hydrocarbons is completely retrievable from the following scheme, written in a most compact way:

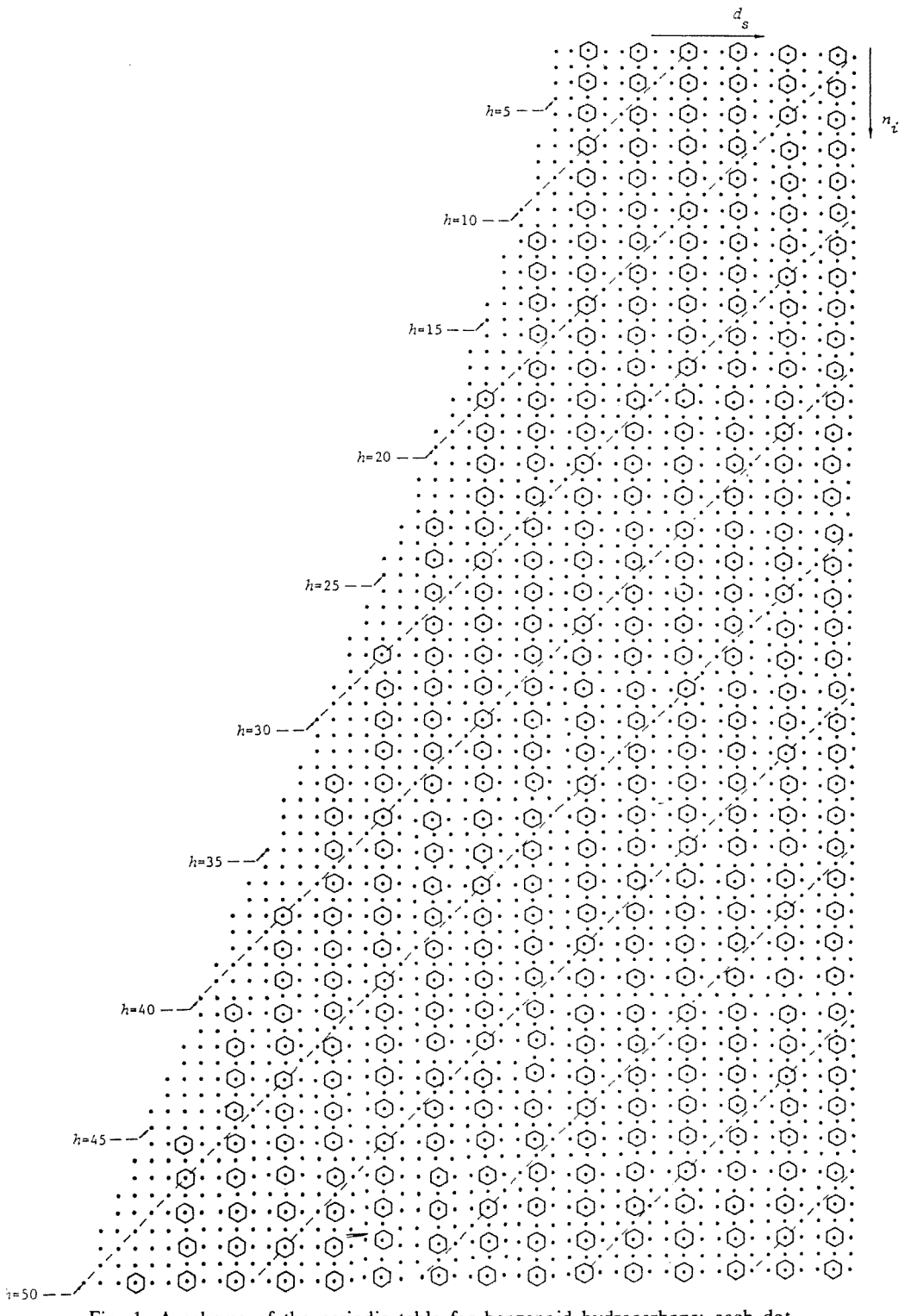

Fig. 1. A scheme of the periodic table for benzenoid hydrocarbons; each dot represents a formula C_nH_s. The existence of all-benzenoids is marked by hexagons.

(I) $C_nH_s(d_s, n_i) \rightarrow C_{n+4}H_{s+2}(d_s + 1, n_i)$

$\downarrow$

$C_{n+3}H_{s+1}(d_s, n_i + 1)$

Upper-left corner (naphthalene): $C_{10}H_8(0, 0)$.

Pericondensed protrusive benzenoids ($h = 1, 2, 3, \ldots$):

$C_{2h+13+3\lceil(12h-3)^{1/2}\rceil}H_{9+\lceil(12h-3)^{1/2}\rceil}$.

The ceiling function $\lceil x \rceil$ is defined as the smallest integer larger than or equal to x. A *protrusive benzenoid* is defined by having a formula C_nH_s with no other formula either to the left or right above it in the periodic table.

3. Periodic table for all-benzenoid hydrocarbons

It is recalled that an all-benzenoid (also called "fully benzenoid") is a Kekuléan benzenoid where all the double bonds of some Kekulé structures belong to aromatic sextets. The possible formulas C_nH_s for all-benzenoids are found among the C_nH_s formulas for benzenoids in general. The all-benzenoid C_nH_s formulas form a regular pattern on the general periodic table, as is shown in fig. 1. For this subset of the formulas the parameter d_s steps by three units, while n_i steps in general by two units. However, for a class of all-benzenoids with fixed h, both d_s and n_i step by six units each. The number of carbon atoms (n) is divisible by six [23,24].

Construct the periodic table for all-benzenoid hydrocarbons by compressing the appropriate C_nH_s formulas (cf. fig. 1) into an array. A portion of this periodic table is given in table 1. The formulas of the table obey the following scheme:

(IIa) $C_nH_s(d_s, n_i) \rightarrow C_{n+12}H_{s+6}(d_s + 3, n_i)$

$\downarrow$

$C_{n+6}H_{s+2}(d_s, n_i + 2)$

Upper-left corner (triphenylene): $C_{18}H_{12}(2, 0)$.

Also the periodic table for all-benzenoid hydrocarbons has a staircase-like boundary as an upper-left edge. The nontrivial problem of this irregular boundary was solved by focusing attention on the so-called *protrusive all-benzenoids*, a subclass of the *extreme all-benzenoids*. The extreme all-benzenoids have formulas along the staircase-like boundary of the periodic table for all-benzenoid hydrocarbons. Furthermore, a protrusive all-benzenoid is an extreme all-benzenoid with a formula having no other formula right above it. Notice that a protrusive all-benzenoid is not

Table 1

Periodic table for all-benzenoid hydrocarbons

d_s							n_i
−7	−4	−1	2	5	8	...	
			$C_{18}H_{12}$	$C_{30}H_{18}$	$C_{42}H_{24}$	...	0
			$C_{24}H_{14}$	$C_{36}H_{20}$	$C_{48}H_{26}$	...	2
			$C_{30}H_{16}$	$C_{42}H_{22}$	$C_{54}H_{28}$	...	4
			$C_{36}H_{18}$	$C_{48}H_{24}$	$C_{60}H_{30}$	...	6
			$C_{42}H_{20}$	$C_{54}H_{26}$	$C_{66}H_{32}$	...	8
			$C_{48}H_{22}$	$C_{60}H_{28}$	$C_{72}H_{34}$	...	10
		$C_{42}H_{18}$	$C_{54}H_{24}$	$C_{66}H_{30}$	$C_{78}H_{36}$	...	12
		$C_{48}H_{20}$	$C_{60}H_{26}$	$C_{72}H_{32}$	$C_{84}H_{38}$	...	14
		$C_{54}H_{22}$	$C_{66}H_{28}$	$C_{78}H_{34}$	$C_{90}H_{40}$	...	16
		$C_{60}H_{24}$	$C_{72}H_{30}$	$C_{84}H_{36}$	$C_{96}H_{42}$	...	18
		$C_{66}H_{26}$	$C_{78}H_{32}$	$C_{90}H_{38}$	$C_{102}H_{44}$	...	20
	$C_{60}H_{22}$	$C_{72}H_{28}$	$C_{84}H_{34}$	$C_{96}H_{40}$	$C_{108}H_{46}$	...	22
	$C_{66}H_{24}$	$C_{78}H_{30}$	$C_{90}H_{36}$	$C_{102}H_{42}$	$C_{114}H_{48}$	...	24
	$C_{72}H_{26}$	$C_{84}H_{32}$	$C_{96}H_{38}$	$C_{108}H_{44}$	$C_{120}H_{50}$	...	26
	$C_{78}H_{28}$	$C_{90}H_{34}$	$C_{102}H_{40}$	$C_{114}H_{46}$	$C_{126}H_{52}$	...	28
$C_{72}H_{24}$	$C_{84}H_{30}$	$C_{96}H_{36}$	$C_{108}H_{42}$	$C_{120}H_{48}$	$C_{132}H_{54}$	...	30
...	...	...	...	...	...	...	.

a protrusive benzenoid, but it is defined in an analogous way with reference to the two periodic tables in question.

It was found that the pericondensed protrusive all-benzenoids can be generated from the benzenoids having the maximum number of internal vertices for a given h, viz. $n_i = (n_i)_{max}$. For the sake of clarity, the smallest of these systems (extremal animals) are depicted in fig. 2. Let such a system be denoted by A. The pericondensed protrusive all-benzenoids may be generated from the A's by a process we shall refer to as *super-circumscribing*. In other words, the pericondensed protrusive all-benzenoids are obtained by super-circumscribing the A benzenoids with steadily increasing numbers of hexagons ($h = 1, 2, 3, \ldots$). The super-circumscribed A shall also be referred to briefly as super-A. In this way, the *super-benzenoids* are defined, at least for the extreme benzenoids.

Interpret the extreme benzenoid system A as a dualist. Then, if A has n vertices, its dualist has n hexagons. Let this benzenoid with n hexagons be the empty subsystem of an all-benzenoid. This all-benzenoid is the super-circumscribed benzenoid of A or super-A. Figure 3 illustrates the definitions of super-circumscribed A or super-A. It is noteworthy that no matter whether A is Kekuléan or non-Kekuléan, super-A becomes Kekuléan.

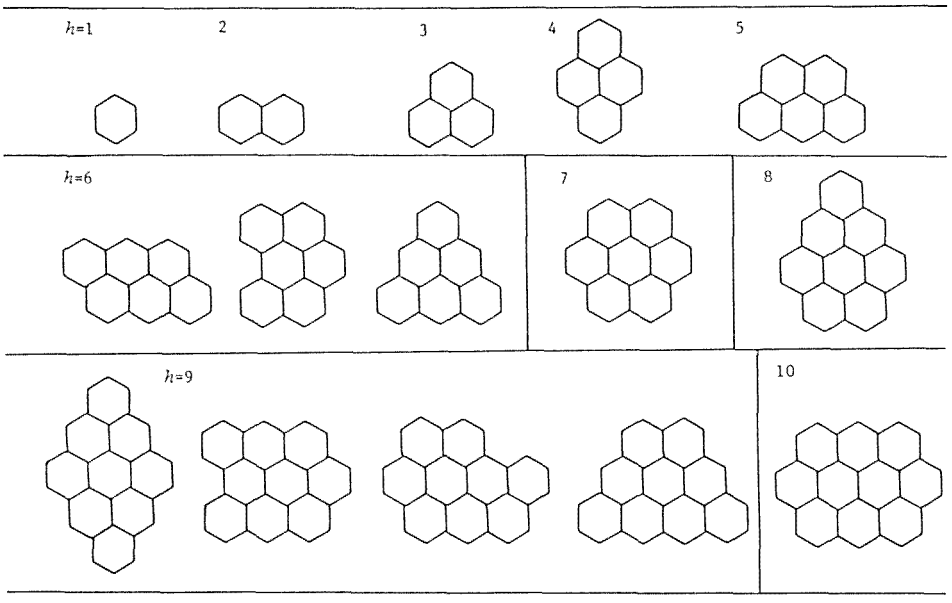

Fig. 2. The smallest ($h \leq 10$) benzenoids with $n_i = (n_i)_{max}$ (extremal animals).

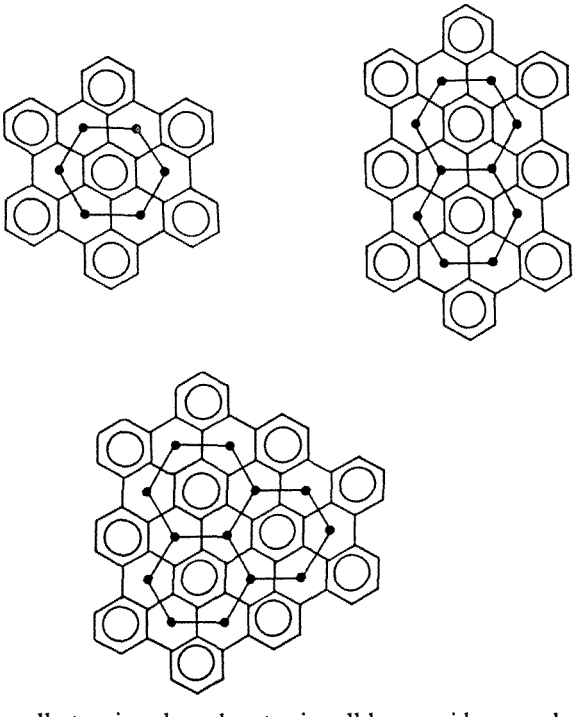

Fig. 3. The three smallest pericondensed protrusive all-benzenoids: super-benzene, super-naphthalene and super-phenalene. The dualists of the empty subsystems are inscribed.

Let a benzenoid A be characterized by the two invariants (h, n_i), where $n_i = (n_i)_{max}$. It has the formula:

(A) $C_{4h-n_i+2}H_{2h-n_i+4}$.

If the super-circumscribed benzenoid of A is characterized by (h^*, n_i^*), then it is found that

$$h^* = 7h - 2n_i + 6, \qquad n_i^* = 10h - 2n_i + 2. \tag{1}$$

Consequently, the following formula for super-circumscribed A is obtained:

(super-A) $C_{4h^*-n_i^*+2}H_{2h^*-n_i^*+4} \equiv C_{18h-6n_i+24}H_{4h-2n_i+14}$.

Furthermore, the Dias parameter of super-A becomes

$$d_s^* = -3h + 2 \tag{2}$$

independent of n_i. It is gratifying to notice that d_s^* steps by three units for every unit of h, as it should in order that no column of the periodic table for all-benzenoid hydrocarbons is skipped.

Table 2

Formulas and invariants for the first pericondensed protrusive all-benzenoids (super-A)

A (h, n_i)[a]	Super-A (h^*, n_i^*)	d_s^*
C_6H_6 (1, 0)	$C_{42}H_{18}$ (13, 12)	– 1
$C_{10}H_8$ (2, 0)	$C_{60}H_{22}$ (20, 22)	– 4
$C_{13}H_9$ (3, 1)	$C_{72}H_{24}$ (25, 30)	– 7
$C_{16}H_{10}$ (4, 2)	$C_{84}H_{26}$ (30, 38)	– 10
$C_{19}H_{11}$ (5, 3)	$C_{96}H_{28}$ (35, 46)	– 13
$C_{22}H_{12}$ (6, 4)	$C_{108}H_{30}$ (40, 54)	– 16
$C_{24}H_{12}$ (7, 6)	$C_{114}H_{30}$ (43, 60)	– 19
$C_{27}H_{13}$ (8, 7)	$C_{126}H_{32}$ (48, 68)	– 22
$C_{30}H_{14}$ (9, 8)	$C_{138}H_{34}$ (53, 76)	– 25
$C_{32}H_{14}$ (10, 10)	$C_{144}H_{34}$ (56. 82)	– 28

[a] See fig. 2.

Table 2 summarizes the derivation of the first ten formulas for pericondensed protrusive all-benzenoids. The formulas for super-A are also obtainable directly from those of A (C_nH_s):

(super-A) $C_{n^*}H_{s^*} \equiv C_{3n+3s+6}H_{2s+6}$.

In conclusion, we find that the periodic table of all-benzenoid hydrocarbons is completely retrievable by means of the scheme (IIa) in addition to:

(IIb) Pericondensed protrusive all-benzenoids ($h = 1, 2, 3, \ldots$):

$$C_{6h+18+6\lceil(12h-3)^{1/2}\rceil}H_{12+2\lceil 12h-3)^{1/2}\rceil}.$$

4. Enumeration results

4.1. BENZENOIDS

The results of enumeration of benzenoid isomers have recently been reviewed and supplemented [17]. That work contains a detailed account of the complete data for $h \leq 10$ and incomplete data for $11 \leq h \leq 44$. Therein, the numbers are given separately according to the *neo* classification (*n* normal; *e* essentially disconnected; *o* non-Kekuléan) and Δ values; cf. e.g. a consolidated report on enumeration of polyhexes [25].

In the present work, a complete enumeration and classification of the benzenoids with $h = 12$ and $h = 13$ was executed with computer aid. Table 3 gives the new data, together with previous data including documentation [3,5,6,10,14,15,19,26–28]. Furthermore, another computer program was used to produce supplementary numbers of benzenoid isomers for $h > 12$. Also these data are found in table 3. In this case, the listing is not complete inasmuch as it does not cover all the possible n_i values for a given h.

4.2. ALL-BENZENOIDS

The all-benzenoid systems have been enumerated up to $h = 10$ by Knop et al. [29] and further on to $h = 18$ by Cyvin et al. [30], who also attained at the numbers of catacondensed all-benzenoids for $h = 19$ and $h = 22$. These numbers are easily split into the numbers for the pertinent isomers when the forms are depicted, as is the case for $h \leq 10$ [29] and $h \leq 13$ [30] in the two publications. Dias [4, 16, 31], in his enumeration of all-benzenoids, concentrated upon the strain-free systems.

Table 4 is a supplemented listing of the known numbers for the isomers of all-benzenoid systems. The distribution into symmetry groups is included.

4.3. SINGLE CORONOIDS

Cyvin and Brunvoll [20] have given a complete list of the numbers of single coronoid isomers (Kekuléan and non-Kekuléan) up to $h = 11$, as obtained with computer aid. At that time, the numbers of catacondensed single coronoids were known up

Table 3

Numbers of benzenoid isomers

h	n_i	Formula	Kekuléan	non-Kekuléan	Total
12	0	$C_{50}H_{28}$	81121[a,b]	0	81121[a,b]
	1	$C_{49}H_{27}$	0	152688[c]	152688[b]
	2	$C_{48}H_{26}$	130665	37653	168318[d]
	3	$C_{47}H_{25}$	0	124119	124119[d]
	4	$C_{46}H_{24}$	57019	17966	74985[d]
	5	$C_{45}H_{23}$	0	38727	38727[d]
	6	$C_{44}H_{22}$	13805	4501	18306[d]
	7	$C_{43}H_{21}$	0	7375[c]	7375[d]
	8	$C_{42}H_{20}$	2085[c]	628[c]	2713[d]
	9	$C_{41}H_{19}$	0	878[c]	878[d]
	10	$C_{40}H_{18}$	213[c]	66[c]	279[d]
	11	$C_{39}H_{17}$	0	61[c]	61[d]
	12	$C_{38}H_{16}$	10[e,f]	3[g]	13[d]
	13	$C_{37}H_{15}$	0	1[g]	1[d]
13	0	$C_{54}H_{30}$	314075[c]	0	314075[c]
	1	$C_{53}H_{29}$	0	648632	648632
	2	$C_{52}H_{28}$	589703	186749	776452
	3	$C_{51}H_{27}$	0	627979	627979
	4	$C_{50}H_{26}$	300833	107952	408785[d]
	5	$C_{49}H_{25}$	0	226837	226837[d]
	6	$C_{48}H_{24}$	83376	30950	114326[d]
	7	$C_{47}H_{23}$	0	50405	50405[d]
	8	$C_{46}H_{22}$	14896	5223	20119[d]
	9	$C_{45}H_{21}$	0	7253[c]	7253[d]
	10	$C_{44}H_{20}$	1836[c]	623[c]	2459[d]
	11	$C_{43}H_{19}$	0	708[c]	708[d]
	12	$C_{42}H_{18}$	139[c]	48[c]	187[d]
	13	$C_{41}H_{17}$	0	35[c]	35[d]
	14	$C_{40}H_{16}$	3[e,f]	1[g]	4[d]
14	0	$C_{58}H_{32}$	1224528[c]	0	1224528[c]
	11	$C_{47}H_{21}$	0	6594	6594[d]
	12	$C_{46}H_{20}$	1471	530	2001[d]
	13	$C_{45}H_{19}$	0	533	533[d]
	14	$C_{44}H_{18}$	89	31	120[d]
	15	$C_{43}H_{17}$	0	16[h]	16[d]
	16	$C_{42}H_{16}$	1[e,f]	0	1[d]

continued . . .

Table 3 (continued)

h	n_i	Formula	Kekuléan	non-Kekuléan	Total
15	13	$C_{49}H_{21}$	0	5612	5612[d]
	14	$C_{48}H_{20}$	1124	446	1570[d]
	15	$C_{47}H_{19}$	0	347	347[d]
	16	$C_{46}H_{18}$	49[h]	21[h]	70[d]
	17	$C_{45}H_{17}$	0	4[h,i]	4[d]
16	15	$C_{51}H_{21}$	0	4501	4502[d]
	16	$C_{50}H_{20}$	790	331	1121[d]
	17	$C_{49}H_{19}$	0	223	223[d]
	18	$C_{48}H_{18}$	22[e,f]	8[g]	30[d]
	19	$C_{47}H_{17}$	0	1[g]	1[d]
17	17	$C_{53}H_{21}$	0	3414	3414[d]
	18	$C_{52}H_{20}$	525	238	763[d]
	19	$C_{51}H_{19}$	0	117	117[d]
	20	$C_{50}H_{18}$	7[e,f]	2[g]	9[d]
18	19	$C_{55}H_{21}$	0	2437	2437[d]
	20	$C_{54}H_{20}$	321	150	471[d]
	21	$C_{53}H_{19}$	0	53	53[d]
	22	$C_{52}H_{18}$	2[e,f]	1[e]	3[d]
19	21	$C_{57}H_{21}$	0	1647	1647[d]
	22	$C_{56}H_{20}$	171	85	256[d]
	23	$C_{55}H_{19}$	0	18[h]	18[d]
	24	$C_{54}H_{18}$	1[j]	0	1[d]
20	23	$C_{59}H_{21}$	0	1009	1009[d]
	24	$C_{58}H_{20}$	88	41	129[d]
	25	$C_{57}H_{19}$	0	4[g]	4[d]
21	25	$C_{61}H_{21}$	0	587	587[d]
	26	$C_{60}H_{20}$	32[h,k]	15[h]	47[d]
	27	$C_{59}H_{19}$	0	1[g]	1[d]
22	27	$C_{63}H_{21}$	0	290	290[d]
	28	$C_{62}H_{20}$	12[e]	4[h,i]	16[d]
23	29	$C_{65}H_{21}$	0	126	126[d]
	30	$C_{64}H_{20}$	3[e]	1[e]	4[d]
24	31	$C_{67}H_{21}$	0	43	4[d]
	32	$C_{66}H_{20}$	1[e]	0	1[d]

[a]Balaban, Brunvoll, Cyvin and Cyvin (1988) [26]. [b]He, He, Wang, Brunvoll and Cyvin (1988) [27]. [c]Cyvin and Brunvoll (1990) [19]. [d]Stojmenović, Tošić and Doroslovački (1986) [10]. [e]Dias (1984) [14]. [f]Dias (1984) [15]. [g]Dias (1986) [5]. [h]Brunvoll and Cyvin (1990) [17]. [i]Dias (1990) [28]. [j]Dias (1982) [3]. [k]Dias (1990) [6].

Table 4

Numbers of all-benzenoid isomers, classified according to symmetry

h	n_i	Formula	D_{6h}	D_{3h}	C_{3h}	D_{2h}	C_{2h}	C_{2v}	C_s	Total
1	0	C_6H_6	1							1[a]
4	0	$C_{18}H_{12}$	0	1						1[a]
6	2	$C_{24}H_{14}$	0	0		1				1[a]
7	0	$C_{30}H_{18}$	0	0		1		1		2[a]
8	4	$C_{30}H_{16}$	0	0		0		1		1[a]
9	2	$C_{36}H_{20}$	0	0		0		1	2	3[a]
10	0	$C_{42}H_{24}$	0	1		0		2	3	6[a]
	6	$C_{36}H_{18}$	0	1		0	1	1	0	3[a]
11	4	$C_{42}H_{22}$	0	0		2	0	2	6	10[b]
12	2	$C_{48}H_{26}$	0	0		1	2	3	19	25[b]
	8	$C_{42}H_{20}$	0	0		0	0	2	2	4[b]
13	0	$C_{54}H_{30}$	0	1[b]	1[b]	0	3[b]	7[b]	20[b]	32[b]
	6	$C_{48}H_{24}$	0	0	0	0	0	3	21	24[b]
	12	$C_{42}H_{18}$	1	0	0	0	0	0	0	1[b]
14	4	$C_{54}H_{28}$	0	0	0	0	0	9	82	91
	10	$C_{48}H_{22}$	0	0	0	1	2	3	5	11
15	2	$C_{60}H_{32}$	0	0	0	0	0	5	179	184
	8	$C_{54}H_{26}$	0	0	0	0	2	8	64	74
	14	$C_{48}H_{20}$	0	0	0	0	0	1	0	1
16	0	$C_{66}H_{36}$	0	0	0	0	0	14[b]	158[b]	172[b]
	6	$C_{60}H_{30}$	0	1	0	2	9	14	304	330
	12	$C_{54}H_{24}$	0	0	1	0	0	4	19	24
17	4	$C_{66}H_{34}$	0	0	0	1	11	30	877	919
	10	$C_{60}H_{28}$	0	0	0	0	0	6	207	213
	16	$C_{54}H_{22}$	0	0	0	1	0	2	1	4
18	2	$C_{72}H_{28}$	0	0	0	1	15	19	1471	1506
	8	$C_{66}H_{32}$	0	0	0	0	0	28	1108	1136
	14	$C_{60}H_{26}$	0	0	0	0	7	11	53	71
19	0	$C_{78}H_{42}$	0	0	2[b]	1[b]	19[b]	41[b]	1076[b]	1139[b]
22	0	$C_{90}H_{48}$	0	0	8[b]	0	0	79[b]	7574[b]	7661[b]

[a]Knop, Müller, Szymanski and Trinajstić (1986) [29]. [b]Cyvin, Brunvoll, Cyvin and Gutman (1988) [30].

Table 5

Number of single coronoid isomers

h	n_i	Formula	Kekuléan	non-Kekuléan	Total
12	0	$C_{48}H_{24}$	312[a]	0	312[a]
	1	$C_{47}H_{23}$	0	552	552
	2	$C_{46}H_{22}$	436	144	580
	3	$C_{45}H_{21}$	0	329	329
	4	$C_{44}H_{20}$	104	38	142
	5	$C_{43}H_{19}$	0	37	37
	6	$C_{42}H_{18}$	2	0	2
13	0	$C_{52}H_{26}$	1435[a]	0	1435[a]
	1	$C_{51}H_{25}$	0	2986	2986
	2	$C_{50}H_{24}$	2593	900	3493
	3	$C_{49}H_{23}$	0	2487	2487
	4	$C_{48}H_{22}$	912	354	1266
	5	$C_{47}H_{21}$	0	521	521
	6	$C_{46}H_{20}$	110	48	158
	7	$C_{45}H_{19}$	0	17	17
14	0	$C_{56}H_{28}$	6785[b]	0	6785[b]
	1	$C_{55}H_{27}$	0	15500	15500
	2	$C_{54}H_{26}$	14779	5318	20097
	3	$C_{53}H_{25}$	0	16469	16469
	4	$C_{52}H_{24}$	7050	2928	9978
	5	$C_{51}H_{23}$	0	4777	4777
	6	$C_{50}H_{22}$	1359	610	1969
	7	$C_{49}H_{21}$	0	590	590
	8	$C_{48}H_{20}$	81	33	114
	9	$C_{47}H_{19}$	0	4	4
15	10	$C_{50}H_{20}$	37	14	51
16	12	$C_{52}H_{20}$	10	2	12
17	14	$C_{54}H_{20}$	2	0	2

[a]Balaban et al. (1987) [25]. [b]He, He, Wang, Brunvoll and Cyvin (1988) [27].

to $h = 14$ [3,25,27,32]. In table 5, we give the complete data for $h = 12, 13$ and 14, where all the numbers for the pericondensed ($n_i > 0$) single coronoid isomers are new. These numbers were also obtained with computer aid. Furthermore, table 5 includes the hand-generated results for three classes of single coronoids with $n_i = (n_i)_{max}$.

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