Supplements to Enumeration of Benzenoid and Coronoid Hydrocarbons

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The previous report on enumeration and classification of benzenoids and coronoids is supplemented. Perhaps the most significant contribution is the enumeration of benzenoids with 12 hexagons.

A consolidated report on the enumeration and classification of benzenoid and coronoid systems by fourteen authors has appeared [1]. The interest of enumerations and classifications of this kind, which are performed by computer programming, has increased during the last years. In fact some supplementary data were already under way while the report [1] was in print. This has prompted us to work out the present note.

The original report [1] should be consulted for all definitions and conventions. Here we only wish to repeat that the term polyhexes is used to denote benzenoids and coronoids together. Only single coronoids (one hole) are counted. Also all helicenic systems are excluded.

Data for Benzenoids with $h = 12$

A total enumeration of all nonisomorphic polyhexes with twelve hexagons ($h = 12$) was executed by the Chinese part of the present collaboration. These co-authors have also determined the numbers within the ABCDEF classification. The Norwegian co-authors generated specifically branched catafusenes for h up to 12 [2] and thus confirmed one of the numbers produced in PR China. This confirmation is very significant inasmuch as the computational methods in PR China and Norway are based on entirely different principles. The numbers of $h = 12$ benzenoids with $\Delta = 2$ and 3 were also computed in Norway [3], whence the number for $\Delta = 4$ was known [1]. Hence the number for $\Delta = 1$ could be taken by subtraction with the aid of results from PR China.

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The main numerical data are given below.

Benzenoids (+ coronoids)	$h = 12$	
Branched catacondensed	68 925	(1)
Total catacondensed	81 121	(2)
Kekuléan pericondensed	203 797	(3)
Non-Kekuléan	384 666	(4)
Total pericondensed	588 463	(5)
Total benzenoids	669 584	(6)
Total polyhexes (benzenoids + coronoids)	671 538	(7)

The number (1) supplements Table 1 (here and throughout we refer to the tables of the consolidated report [1]). The next number (2) should also be entered into Table 1, as well as into Table 8 (for $n_i = 0$) and Table 10. The numbers (3), (4) and (5) fit into Table 2, while (4) also goes into Table 5 (under o). With regard to the important number (6) it should be entered into Tables 5 and 10. Finally (7) goes into Table 5.

In spite of this enumeration it is still unknown how many $h = 12$ benzenoids are normal (***n***) and how many essentially disconnected (***e***). This is of relevance to the "*neo*" classification (cf. Table 5). It can only be deduced that the sum ($\boldsymbol{n} + \boldsymbol{e}$) for $h = 12$ is 284 918.

Coronoids

Some of the main data for coronoids have also been extended to higher h values. Thus Table 3 (catacondensed coronoids) is supplemented with the number 15 417 for primitive coronoids of $h = 21$. Furthermore one has 6745 annelated (branched) systems for $h = 14$, which gives a total catacondensed of 6785.

Table 4 is supplemented with the following data for systems with 13 hexagons:

Coronoids	$h = 13$
Pericondensed Kekuléan	3 615
Non-Kekuléan	7 313 [4]
Total pericondensed	10 928

These numbers are consistent with a total number of coronoids of $h = 13$ amounting to 12 363 [4, 5]. This number should be entered in parentheses (because it pertains to coronoids) into Table 5 together with (7313) under the label o. It is noted that the separate numbers of $h = 13$ normal pericondensed ($\boldsymbol{n}\,\boldsymbol{p}$) and essentially disconnected (***e***) coronoids are still unknown. Only their sum ($\boldsymbol{n}\,\boldsymbol{p} + \boldsymbol{e}$) is now established to be 3615.

Another piece of information for $h = 14$ coronoids was deduced: there are 23 270 pericondensed Kekuléan coronoid systems with 14 hexagons.

Symmetry

Several specific enumerations of polyhexes with hexagonal symmetry have been performed [5, 6]. Below we give some data in continuation of Table 6.

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Benzenoids	D_{6h}	C_{6h}
$h = 25$	3[a]	8[a]
31	5[a]	32[a]
37	8[a]	128[a]
43	13[a]	527[a]
49	20[a]	2209[a]
55	35[a]	9470[a]
61	60	[b]
67	104	[b]
73	183	[b]

[a] Ref. [6]. [b] Unknown.

Coronoids: $h =$	24	30	36	42	48	54	60
D_{6h}	9[a]	20[a]	47[a]	97[a]	222	459	1029
C_{6h}	7[a]	44[a]	225[a]	1113[a]	[b]	[b]	[b]

[a] Ref. [5]. [b] Unknown.

Δ Values

Table 7 deals with the numbers of polyhexes classified according to Δ values. Here we give the available supplements for benzenoids [3] along with original data for coronoids (figures in parentheses).

Benzenoids (coronoids)	$h = 12$	$h = 13$	$h = 14$
$\Delta = 0$	285016	[b] (5050)	[b] (30055)
$\Delta = 1$	320859	[b] (5913)	[b] ([b])
$\Delta = 2$	60705	[b] (1301)	[b] ([b])
$\Delta = 3$	2990	21675 (98)	[b] ([b])
$\Delta = 4$	14[a]	211 (1)	2588 ([b])

[a] Ref. [1]. [b] Unknown.

Finally it was also derived that there are 48 benzenoids with $h = 15$ and $\Delta = 5$.

From the data which have been reported it may be deduced that there are 8 concealed non-Kekuléan ($K = 0$, $\Delta = 0$) benzenoids with $h = 11$ [7]. In the same way it is implied that there are 98 concealed non-Kekuléans with $h = 12$ [8].

Internal Vertices

With regard to Table 8 it was already mentioned that the present results provide the supplementary figure for $n_i = 0$ at $h = 12$. Consequently, the corresponding figure for $n_i = 1$ is obtainable by subtraction. It reads 152688.

The ABCDEF Classification

Finally we give supplementary data to Table 9. They pertain to systems with 12 hexagons.

Benzenoids (coronoids)	$h = 12$	
	A: Kekuléan	Non-Kekuléan
B	12196[a]	
C	68925	
D	3066 (135)	7170 (176)
E	(11)[a]	
F	200731 (708)	377496 (924)

[a] Ref. [1].

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