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Enumeration and Classification of Double Coronoid Hydrocarbons Appendix: Triple Coronoids

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An enumeration of double coronoids (polyhexes with two holes) is performed, both by hand and by computer. The numbers 15123 and 125760 for the systems with $h = 17$ and $h = 18$, respectively, are reported for the first time. Here h denotes the number of hexagons. The generated systems are classified in different ways. In this connection the strata of corona hole constellations are defined, depending on the proximity of the holes. As appendix, a first enumeration of triple coronoids is reported.

INTRODUCTION

It seems clear that the coronoids can no longer be circumvented in reviews and monographs which deal with polyhexes[1-7], these geometrical figures consisting of congruent regular hexagons in a plane. Coronoid (systems) are polyhexes with holes, referred to as corona holes. The systems correspond to conjugated (polycyclic aromatic) hydrocarbons in organic chemistry. A corona hole should have a size of at least two hexagons. When it is interpreted as a polyhex, we may speak about the naphthalene hole, phenalene hole, anthracene hole, *etc.* Kekulene for instance, which has been synthesized in a celebrated work[8], corresponds to a coronoid with the coronene hole.

A polyhex with more than one corona hole is called a multiple coronoid, in contrast to a single coronoid which has exactly one hole. In some recent theoretical works[9-12] allowance was made for several holes. The number of holes is referred to as the genus[10] and identified by the symbol g.

Generation and enumeration of polyhexes has attracted the interest of many investigators.[13-16] In these reports the extensive work done on enumerations of polyhexes without holes and of single coronoids is well documented. The corresponding investigations of multiple coronoids, on the other hand, have started only very recently.

The present work is a continuation of our generation and enumeration work for double coronoids ($g = 2$). Results for the systems with $h > 16$ are reported for the first time, where h is used to designate the number of hexagons. Furthermore, the first results for triple coronoids ($g = 3$) are given as an appendix.

PREVIOUS RESULTS FOR DOUBLE CORONOIDS

The first computerized generation and enumeration of multiple coronoids is due to Knop *et al.*[17], who published their material for $h = 13$ and 14. The numbers are found in Table I under $g = 2$. The unique system for $h = 13$ was, perhaps for the first time, depicted by Dias[18], who inferred that it is the smallest double coronoid, but did not state explicitly that it is the only one with that number of hexagons. Knop *et al.*[17] recognized this system among the totality of 3210620 polyhexes. Similary they deduced the 11 double coronoids by recognition from 15443871 generated polyhexes. The 12 forms for $h \leq 14$ are depicted in the mentioned work.[17] The computations were extended to $h = 15$ in two parallel works published together.[19] Herein the 149 double coronoids with $h = 15$ were deduced both by recognition from 74662005 systems and by a specific generation.[21] Pictures of the forms are given. Finally, the Düsseldorf-Zagreb group recognized 1618 double coronoids from the formidable number of 362506902 polyhexes with $h = 16$, a computation which lasted uninterupted for about 3 months.[20]

TABLE I

Numbers of nonisomorphic planar polyhexes

h	g 0	1	2
13	3198256	12363	1
14	15367577	76283	11
15	74207910*	453946	149
16	359863778*	2641506*	1618

* Ref. 20; otherwise, see the text.

MAIN PRINCIPLES

Previously described computer programs[21,22] were employed for a specific generation, rather than recognition,[21] of double coronoid systems. In other words, only double coronoids were generated.

Firstly, nonisomorphic systems with $h + 1$ hexagons were produced by adding one hexagon at a time to all the double coronoids with h hexagons. Hexagons were added into all possible positions to the outer perimeter only, never into the corona holes.

Secondly, the necessary extra systems, not obtained by the described additions of hexagons, were supplemented after each run for a given h value.

The extra systems of the latter category were generated by hand in the first analysis of this kind.[19] In the present work this generation is supported by a computer-aided analyses.

MAIN RESULT

Table II shows the enumeration results for double coronoids. The number of systems emerging from additions to double coronoids with different h values are listed in separate columns. The number of extra systems are found at the top of each column, i.e. along the diagonal 1, 6, 15, ...

The results include the numbers of all nonisomorphic double coronoids up to h = 18.

TABLE II

Numbers of nonisomorphic planar double coronoids

	h value of the starting system					
h	13	14	15	16	17	18
13	1					
14	5	6				
15	56	78	15			
16	421	891	242	64		
17	3128	7759	2821	1209	206	
18	20929	59619	25431	14894	4159	728

CLASSIFICATION OF THE DOUBLE CORONOIDS

After having computer-generated the double coronoid systems they were divided into different classes by recognition. Table III gives a survey. The systems were classified according to Δ values. Here Δ is the color excess,[7] which signifies the absolute magnitude of the difference between the numbers of black and white vertices.[1,16] The "*neo*" classification[16] implies the normal (n), essentially disconnected (e) and non-Kekuléan (o) systems. Precise definitions are found in some of the works cited above.[5,7,16] Also the distribution into symmetry groups is indicated. Here it should be noted that only four symmetry groups, viz. D_{2h}, C_{2h}, C_{2v} *and* C_s are possible for double coronoids, out of the eight possible groups for polyhexes in general. Double coronoids can never have trigonal or hexagonal symmetry.

TABLE III

Numbers of double coronoids according to different classifications

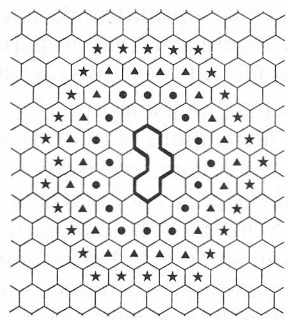
h	Type*	Δ	D_{2h}	C_{2h}	C_{2v}	C_s	Total
13	*n*	0	1	0	0	0	1
14	*n*	0	0	2	3	2	7
	o	1	0	0	0	4	4
15	*n*	0	3	4	10	53	70
	e	0	0	1	1	0	2
	o	1	0	0	2	65	67
	o	2	0	0	1	9	10
16	*n*	0	3	23	30	596	652
	e	0	0	3	3	20	26
	o	1	0	0	5	765	770
	o	2	0	0	4	156	160
	o	3	0	0	0	10	10
17	*n*	0	9	43	116	5370	5538
	e	0	0	8	9	320	337
	o	0	1	0	0	0	1
	o	1	0	0	21	7217	7238
	o	2	0	0	20	1816	1836
	o	3	0	0	2	166	168
	o	4	0	0	0	5	5
18	*n*	0	9	191	287	41900	42387
	e	0	0	47	25	3874	3946
	o	0	0	2	4	5	11
	o	1	0	0	52	60157	60209
	o	2	0	0	48	17041	17089
	o	3	0	0	9	2027	2036
	o	4	0	0	1	80	81
	o	5	0	0	0	1	1

* Abbreviations: *e* essentially disconnected: *n* normal; *o* non-Kekuléan.

THE EXTRA DOUBLE CORONOIDS WITH $h = 17$

Introductory Remarks

In the derivation of the new number for $h = 17$ double coronoids (see Table II) the crucial point was to identify the extra systems, i.e. those which are not obtained by addition of one hexagon to the outer perimeter of any double coronoid with $h = 16$. A listing of these $h = 17$ extra systems starts with all possible corona hole constellations which are compatible with this number of hexagons for the double coronoid. In this connection we shall speak about different strata, referring to the positions which two corona holes may assume in relation to each other. If the holes are as close as possible to each other, the constellation is said to be of the first stratum. The next-nearest positions are of the second stratum, and so on. In order to make this point clear we have marked in the diagram below the appropriate positions around the phenanthrene hole by black circles, triangles and asterisks according to their proximity to the hole.



Now, a constellation of the first stratum (str = 1) emerges when the second hole occupies a hexagon marked with a circle, one of the second stratum (str = 2) comes up when the second hole occupies a triangle, but not a circle, and so on.

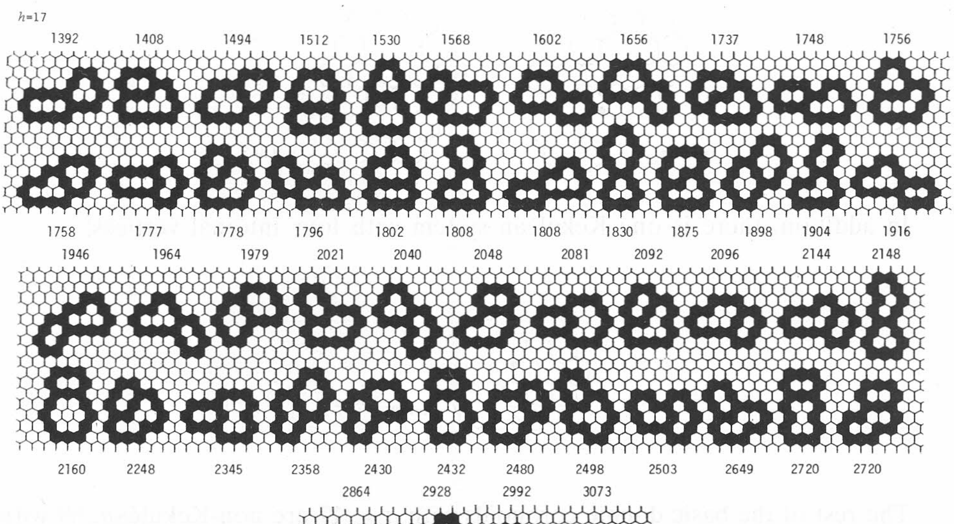


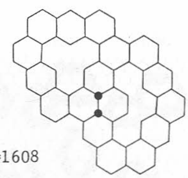
Figure 1. The 50 nonisomorphic primitive double coronoids with h = 17. They are ordered according to increasing K numbers (see the text).

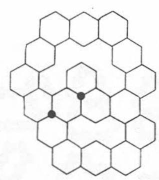
First Stratum

A constellation of two corona holes of the first stratum determines uniquely the smallest double coronoid with these two holes. Such a system we shall call a *basic* double coronoid, in analogy with basic single coronoids possessing one hole each. A basic double coronoid which is catacondensed and has exactly two branching hexagons, is called *primitive.* Again, this class is a generalization of the primitive single coronoids.[7,21] In other words, a primitive double coronoid consists of two primitive single coronoids linked together so that no pericondensation occurs. The two single coronoids must have some (at least two) hexagons in common.

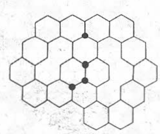
In Figure 1 all the generated (nonisomorphic) primitive double coronoids are depicted. In order to increase the amount of information they are supplied with Kekulé structure counts (K). These K numbers were obtained from a computer program using the determinant of the adjacency matrix or, when necessary, the Pfaffian of a skew-symmetric adjacency matrix. The adaptation of these methods to single coronoid systems is explained in some detail elsewhere.[23] In the present work a generalization of the program for multiple coronoids was produced. There are exactly 50 nonisomorphic primitive double coronoids with h = 17 (cf. Figure 1).

Among the non-primitive basic double coronoids with h = 17 we find exactly 40 Kekuléan systems with two internal vertices each. For the sake of brevity we do not reproduce all the forms here, but we show two examples below.

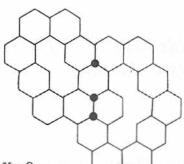

K=1608

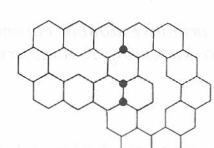

K=1348

In addition, there is one Kekuléan system with four internal vertices:


K=1191

The rest of the basic double coronoids with h = 17 are non-Kekuléan: 69 with Δ = 1 and 6 with Δ = 2. In the former class (Δ = 1) 67 systems have one internal vertex each, while the following 2 systems have three.


K=0


K=0

The mentioned systems with Δ = 2 are depicted in Figure 2.

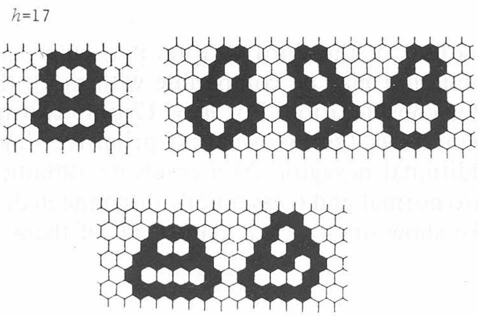


Figure 2. The 6 nonisomorphic basic double coronoids with h = 17 and Δ = 2. Each of them has two internal vertices.

The above survey accounts for the 166 basic double coronoids with $h = 17$.

Second Stratum

A phenalene hole and a naphthalene hole in constellations of the second stratum give double coronoids with $h = 17$. There are 12 such combinations and no other possibilities. The systems in question are depicted in Figure 3. We find 10 Kekuléans among them and 2 non-Kekuléans with $\Delta = 1$.

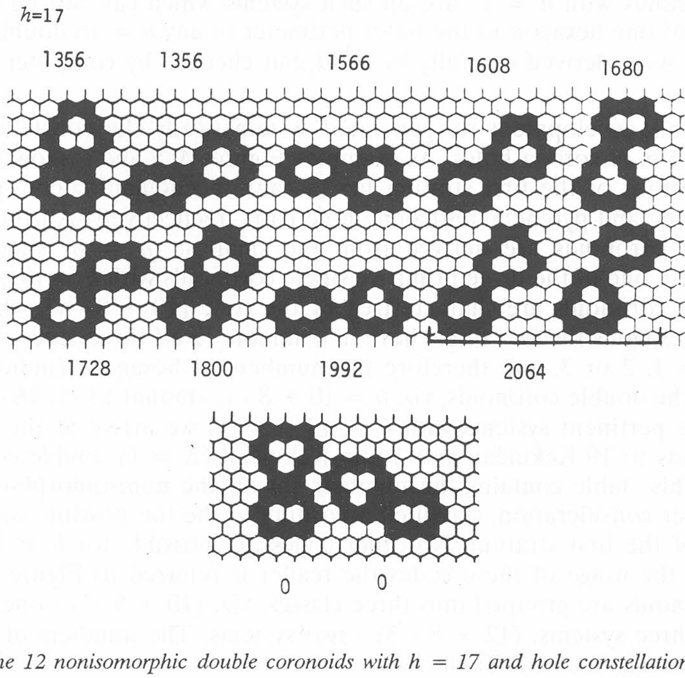
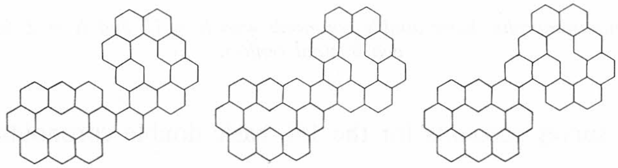


Figure 3. The 12 nonisomorphic double coronoids with h = 17 and hole constellations of str = 2

Third Stratum

For hole combinations of the third stratum particular care must be taken because one hole constellation may be compatible with more than one double coronoid of the type under consideration. For $h = 17$ only two naphthalene holes are of interest in this connection; the two smallest primitive single coronoids ($h = 8$) are linked by one additional hexagon. As a result we obtained 28 systems: 16 Kekuléan, of which 10 are normal and 6 essentially disconnected, and 12 non-Kekuléan with $\Delta = 1$. Below we show one of each classes, all of them having the same hole constellation.



K=2432(n) K=1600(e) K=0(o)

Systematic Generations

How do we know that the 166 (str = 1) + 12 (str = 2) + 28 (str = 3) = 206 double coronoids with $h = 17$ are all such systems which can not be obtained by an addition of one hexagon to the outer perimeter of any $h = 16$ double coronoid? The systems were derived carefully by hand, but checked by computer-assisted generations.

Under this development we generated systematically the constellations for a number of pairs of corona holes. As examples Figures 4, 5 and 6 show the schemes for constellations of the first stratum for the anthracene/naphtalene, phenanthrene/naphthalene and pyrene/naphthalene hole pairs, recpectively. All the corresponding double coronoids are derived from the smallest ($h = 8$) single coronoid combined with one of the three primitive single coronoids with $h = 10$. Accordingly, these double coronoids are characterized by the code (10 + 8 - x), where x is the number of hexagons the two single have in common. In all three cases (Figures 4-6) one has x = 1, 2 or 3, and therefore the numbers of hexagons (indicated on the Figures) of the double coronoids, viz. $h = 10 + 8 - x$, amount to 15, 16 or 17. When counting the pertinent systems with $h = 17$ ($x = 1$) we arrive at the number 21. It corresponds to 19 Kekuléan and 2 non-Kekuléan ($\Delta = 1$) double coronoids; cf. Table IV. This table contains the numbers for all the nonisomorphic double coronoids under consideration, classified according to the ten possible codes for constellations of the first stratum. No other codes are possible for $h = 17$. In order to illustrate the usage of these codes the reader is referred to Figure 2. Here the double coronoids are grouped into three classes, viz. (10 + 9 -2) - one system; (11 + 8 - 2) - three systems; (12 + 8 - 3) - two systems. The numbers of systems are seen to be consistent with Table IV.

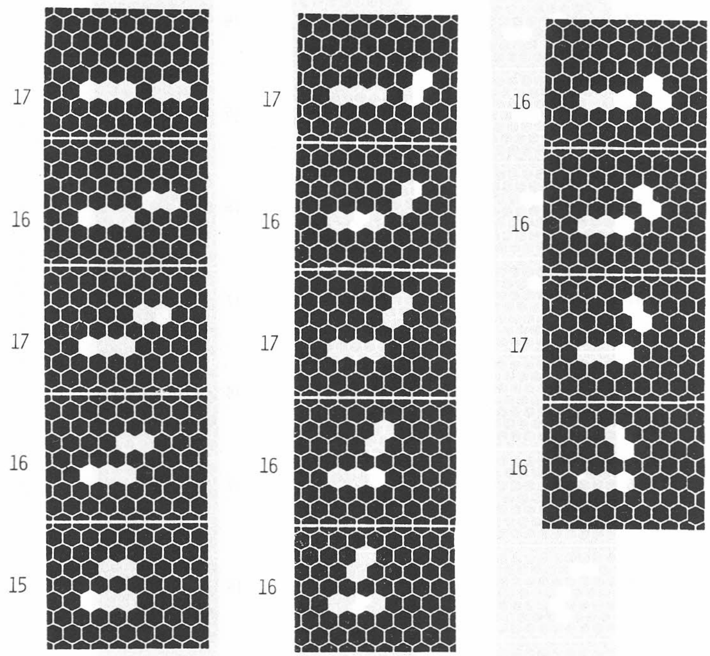


Figure 4. All nonisomorphic constellations of the first stratum for the anthracene/naphthalene pair of corona holes.

The principles of systematic generations, where advantage was taken of the different codes, were used in the analysis by hand. Parallel with this, a computer program was designed using somewhat different principles. Here the double coronoids were grouped according to the numbers of hexagons of the corona holes, say h_1^0 and h_2^0. We use the symbol h_1^0/h_2^0 for $str = 1$, $h_1^0//h_2^0$ for $str = 2$, *etc.* Thus, for instance, the systems of Figures 4 and 5 are to be classified as 2/3, while those of Figure 6 belong to 2/4. Table V is the result of the computer analysis for $h = 17$ when $str = 1$. The distribution into symmetry groups is included, just as in Table IV. The individual numbers are seen to be different from those of Table IV (because of the different classifications), but they should add up to the same totals. Indeed, from both Table IV and Table V one obtains the following summary.

$h = 17$, $str = 1$

Δ	C_{2h}	C_{2v}	C_s	Total
0	4	17	70	91
1	0	1	68	69
2	0	2	4	6

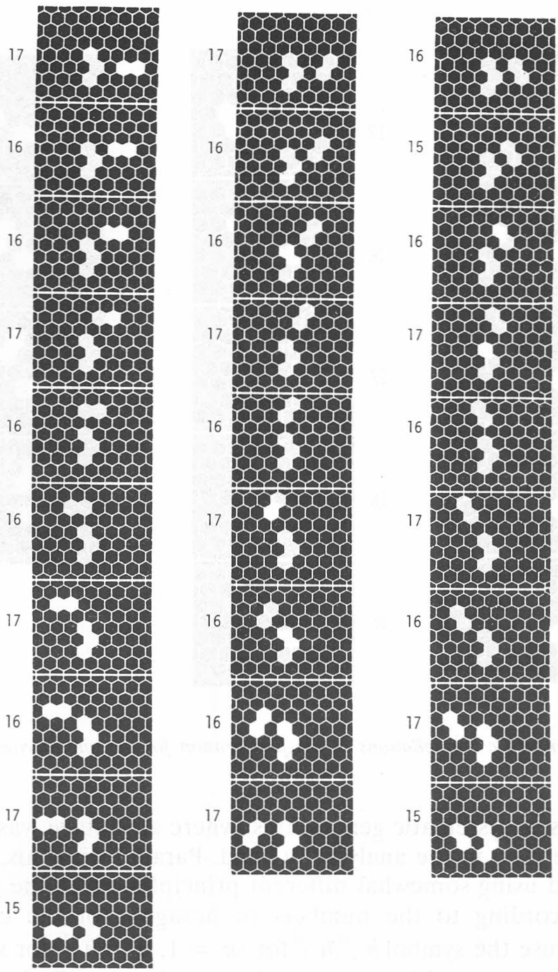


Figure 5. All nonisomorphic constellations of the first stratum for the phenanthrene/naphthalene pair of corona holes.

For *str* > 1 the two classification schemes (codes and number of hexagons in holes) coincide. The following result was obtained, both from the analysis by hand and the computer program.

$h = 17$

str	Code	Holes	Δ	D_{2h}	C_{2h}	C_{2v}	C_s	Total
2	(9+8−0)	2//3	0	0	0	0	10	10
			1	0	0	1	1	2
3	(8+8+1)	2///2	0	1	3	6	6	16
			1	0	0	0	12	12

TABLE IV

Numbers of h = 17 basic double coronoids (I)

Code	Δ	C_{2h}	C_{2v}	C_s	Total
(9+9−1)	0	1	1	0	2
(10+8−1)	0	0	3	16	19
	1	0	0	2	2
(10+9−2)	0	0	1	9	10
	1	0	0	11	11
	2	0	1	0	1
(11+8−2)	0	0	0	20	20
	1	0	0	24	24
	2	0	0	3	3
(10+10−3)	0	3	5	3	11
	1	0	0	7	7
(11+9−3)	0	0	1	2	3
	1	0	0	5	5
(12+8−3)	0	0	5	12	17
	1	0	1	19	20
	2	0	1	1	2
(11+10−4)	0	0	1	3	4
(12+9−4)	0	0	0	1	1
(13+8−4)	0	0	0	4	4

TABLE V

Numbers of h = 17 basic double coronoids (II)

h_1^0/h_2^0	Δ	C_{2h}	C_{2v}	C_s	Total
2/3	0	0	2	12	14
	1	0	0	2	2
2/4	0	0	2	22	24
	1	0	1	22	23
	2	0	1	3	4
2/5	0	0	2	14	16
	1	0	0	17	17
	2	0	0	1	1
2/6	0	0	1	4	5
	1	0	0	4	4
2/7	0	0	1	0	1
3/3	0	3	4	8	15
	1	0	0	12	12
	2	0	1	0	1
3/4	0	0	2	9	11
	1	0	0	10	10
3/5	0	0	2	1	3
	1	0	0	1	1
4/4	0	1	1	0	2

TABLE VI

Numbers of h = 18 basic double coronoids (I)

Code	Δ	D_{2h}	C_{2h}	C_{2v}	C_{2s}	Total
(10+9−1)	0	0	0	0	12	12
	1	0	0	0	1	1
(11+8−1)	0	0	0	0	26	26
	1	0	0	0	4	4
(10+10−2)	0	2	8	3	23	36
	1	0	0	0	32	32
	2	0	0	1	2	3
(11+9−2)	0	0	0	0	14	14
	1	0	0	0	17	17
	2	0	0	1	1	2
(12+8−2)	0	0	0	0	74	74
	1	0	0	0	88	88
	2	0	0	0	11	11
(11+10−3)	0	0	0	0	20	20
	1	0	0	0	29	29
(12+9−3)	0	0	0	2	9	11
	1	0	0	1	18	19
	2	0	0	1	1	2
(13+8−3)	0	0	0	3	31	34
	1	0	0	0	46	46
	2	0	0	2	8	10
(11+11−4)	0	1	3	1	2	7
(12+10−4)	0	0	0	1	12	13
	1	0	0	1	7	8
(13+9−4)	0	0	0	0	4	4
(14+8−4)	0	0	0	0	15	15
	1	0	0	0	4	4

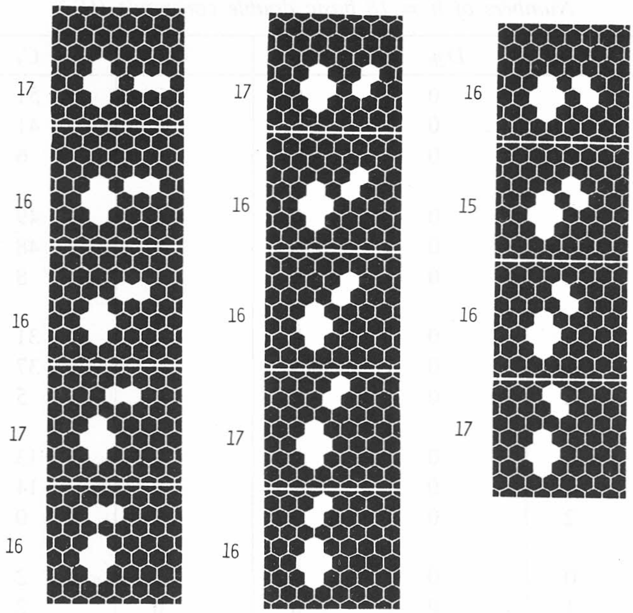


Figure 6. All nonisomorphic constellations of the first stratum for the pyrene/naphthalene pair of corona holes.

DOUBLE CORONOIDS WITH h = 18

The analyses, with and without computer aid, were extended to double coronoids with $h = 18$ using the same principles as outlined above. The results are reported just briefly in the following.

Numbers of the basic double coronoids ($str = 1$) are found in Table VI and VII. A summary from either of these tables reads:

$h = 18$, $str = 1$

Δ	D_{2h}	C_{2h}	C_{2v}	C_s	Total
0	3	11	10	242	266
1	0	0	2	246	248
2	0	0	5	23	28

For $str > 1$ we only give a summary of the results, which were obtained by the two approaches: hand-generation by means of codes and computer-generation according to size of the corona holes.

TABLE VII

Numbers of h = 18 basic double coronoids (II)

h_1^0/h_2^0	Δ	D_{2h}	C_{2h}	C_{2v}	C_s	Total
2/4	0	0	0	0	51	51
	1	0	0	0	41	41
	2	0	0	0	6	6
2/5	0	0	0	1	49	50
	1	0	0	0	48	48
	2	0	0	1	8	9
2/6	0	0	0	1	31	32
	1	0	0	0	37	37
	2	0	0	0	5	5
2/7	0	0	0	0	13	13
	1	0	0	0	14	14
	2	0	0	1	0	1
2/8	0	0	0	1	2	3
	1	0	0	0	2	2
3/3	0	1	6	3	20	30
	1	0	0	0	18	18
	2	0	0	0	2	2
3/4	0	0	0	0	40	40
	1	0	0	2	49	51
	2	0	0	2	2	4
3/5	0	0	0	1	21	22
	1	0	0	0	21	21
	2	0	0	1	0	1
3/6	0	0	0	1	6	7
	1	0	0	0	4	4
3/7	0	0	0	1	0	1
4/4	0	1	5	1	5	12
	1	0	0	0	10	10
4/5	0	0	0	0	4	4
	1	0	0	0	2	2
5/5	0	1	0	0	1	1

$h = 18$

str	Δ	D_{2h}	C_{2h}	C_{2v}	C_s	Total
2	0	0	5	5	61	71
	2	0	0	3	9	12
3	0	0	0	0	15	15
	1	0	0	0	26	26
	2	0	0	3	6	9
4	0	1	7	1	20	29
	1	0	0	0	24	24

CONCLUSION AND APPENDIX

This work gives a significant supplement to the previously known numbers of double coronoids (cf. Table I). As the gross totals of nonisomorphic double coronoids we arrived at 15123 systems with $h = 17$ and 125760 systems with $h = 18$.

Triple coronoids ($g = 3$) are found for $h \geq 18$. They were enumerated for $h = 18$ and $h = 19$, resulting in the gross totals of 4 and 71, respectively. For these systems also the trigonal symmetries (D_{3h} and C_{3h}) are possible (in addition to D_{2h}, C_{2h}, C_{2v} and C_s), but not hexagonal (D_{6h} and C_{6h}). It was arrived at the following classifications.

$g = 3$

h	Δ	D_{3h}	C_{3h}	D_{2h}	C_{2v}	C_s	Total
18	0	0	0	1	1	0	2
	1	0	1	0	0	1	2
19	0	1	0	0	8	24	33
	1	0	0	0	0	31	31
	2	0	0	0	0	6	6
	3	0	1	0	0	0	1

The 4 systems with $h = 18$ are depicted in Figure 7. The calculated K numbers for the two Kekuléan ($\Delta = 0$) systems are given therein. These two double coronoids are catacondensed, and they are classified as primitive according to a natural ge-

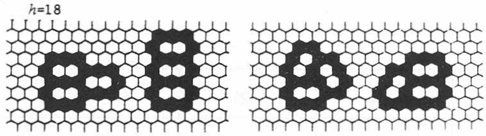


Figure 7. The 4 nonisomorphic triple coronoids with h = 18.

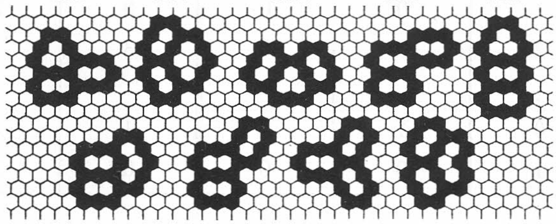


Figure 8. The 9 nonisomorphic primitive triple coronoids with h = 19.

neralization of this concept. Among the Kekuléan triple coronoids with $h = 19$ there are nine (catacondensed) primitive systems. Their forms, along with K numbers, are shown in Figure 8.

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SAŽETAK

Prebrojavanje i klasifikacija dvostrukih koronoidnih ugljikovodika

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Provedeno je prebrojavanje dvostrukih koronoidnih ugljikovodika. Po prvi puta prebrojeni su koronoidni sustavi sa 17 i 18 benzenskih prstenova. Predložena je također i klasifikacija tih ugljikovodika. U dodatku je po prvi put provedeno prebrojavanje trostrukih koronoidnih ugljikovodika.