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CORONENIC CORONOIDS: A COURSE IN CHEMICAL ENUMERATION

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Abstract: A coronenic coronoid has a coronene corona hole. This work deals mainly with circular benzenoids, each perforated by exactly one coronene hole. Complete mathematical solutions are reported for the numbers of C_nH_s isomers for these systems. They are presented as explicit combinatorial formulas on one hand and in terms of generating functions on the other. Finally some general formulations (in three "pictures") are given for the C_nH_s formulas of the systems under consideration, viz. the coronenic perforated circular benzenoids.

Introduction. The first one of the two coronoid hydrocarbons which have been synthesized [1,2], viz. kekulene [2–4], is coronenic.

Definition: A coronenic coronoid is a coronoid [5,6] with only coronene(s) as the corona hole(s).

In the fractal polyhex systems [7] (see also the preceding article) the coronene hole occurs very frequently. Many of these fractal systems are "laceflowers" [8], viz. multiple coronoids with hexagonal symmetry. All laceflowers with D_{6h} symmetry and h (number of hexagons) $\leq$ 49 have been generated. Coronene holes do occur among them, but they are not coronenic since there is no system among them with exclusively coronene holes. However, a coronenic laceflower is encountered already on pursuing the generation one step further, to $h = 54$; see Fig. 1. If there are no inadvertent omissions in these generations, one has the following enumeration result: there are 1, 1, 2, 4, 8, 10 and 26 laceflowers with D_{6h} symmetry and h = 36, 37, 42, 43, 48, 49 and 54, respectively.

In the remaining of this paper it is tacitly assumed that the term "coronoid"

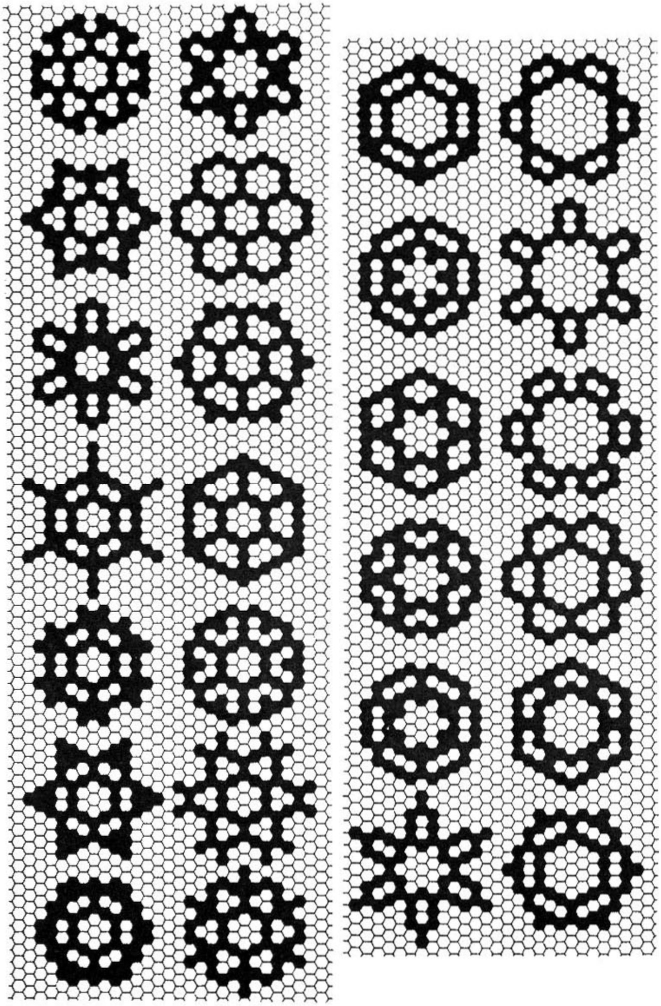

Fig. 1. All laceflowers with D_{6h} symmetry and $h = 54$.

refers to a system with exactly one hole (strictly speaking a single coronoid).

Circular Benzenoids. The circular benzenoids [9,10], **O**, exhibit six characteristic shapes, which are identified by the index $\epsilon = 0, 1, 2, 3, 4, 5$ (cf. Fig. 2). From a set of six ground forms [9–12] all the circular benzenoids are generated by successive circumscribings. It is known that there exists exactly one C_nH_s isomer of each circular benzenoid [9–16].

Perforated Circular Benzenoids. The **O** systems perforated by naphthalene corona holes are studied elsewhere [17]. The subject of the present work are the **O** systems each perforated by a coronene hole: the coronenic perforated circular benzenoids, C. Six of the smallest systems of this category, one for each characteristic shape (ϵ value), are shown in Fig. 2. Except for the two cases $C_{48}H_{24}$ and $C_{53}H_{25}$ there are more than one C_nH_s isomers of the C systems, arising from the different possibilities where to place the coronene hole. In the present work a complete mathematical solution is reported for the numbers of nonisomorphic C_nH_s isomers for C.

Circumscribing. Consider a benzenoid **B** with H hexagons and the formula $C_NH_S \equiv (N;S)$, symbolized by $\mathbf{B} \in \{N;S\}$. Furthermore, write (circum–**B**) $\in \{N_1;S_1\}$ for

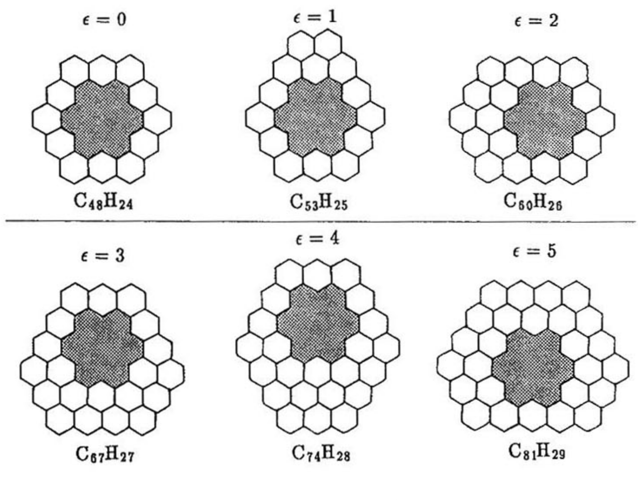

Fig. 2. Smallest coronenic perforated circular benzenoids.

circumscribed **B**, which is assumed to hold H_1 hexagons. This circumscribing adds S hexagons to **B**, hence $H_1 = H + S$, while $S_1 = S + 6$. From the known relations between invariant of benzenoids [18], especially

$$H = \tfrac{1}{2}(N - S) + 1 \tag{1}$$

it was arrived at [9–11]

$$(N_1;S_1) = (N + 2S + 6;\ S + 6) \tag{2}$$

Assume now (k–circum–**B**) $\in \{N_k;S_k\}$. Then, on repeated application of the formula (2) for $(N_1;S_1)$ it was obtained [9,10]

$$(N_k;S_k) = (6k^2 + 2kS + N;\ 6k + S) \tag{3}$$

Associated Benzenoid. The associated benzenoid to a coronoid C is defined by the benzenoid which emerges when the corona hole of C is completely filled by hexagons. Let C be a coronenic coronoid with the formula $C_nH_s \equiv (n;s)$: C $\in \{n;s\}$. Furthermore, let C $\in \{N;S\}$ be the associated benzenoid to C. Then the following connection is valid for the coefficients of C_nH_s and C_NH_S.

$$(n;s) = (N - 6;\ S + 6) \tag{4}$$

Coronenic Perforated Polycircumpyrenes. The title systems were chosen as examples. The smallest such system is found in Fig. 2 ($C_{74}H_{28}$; $\epsilon = 4$). It is a perforated dicircumpyrene. The $(k+2)$–circumpyrenes are considered, where $k = 0, 1, 2, \ldots$; $k = 0$ pertains to dicircumpyrene. In the following, the numbers of nonisomorphic C_nH_s isomers for the coronenic $(k+2)$–circumpyrenes are determined analytically by different methods. The problem reduces to finding the numbers of distinct positions for the coronene hole.

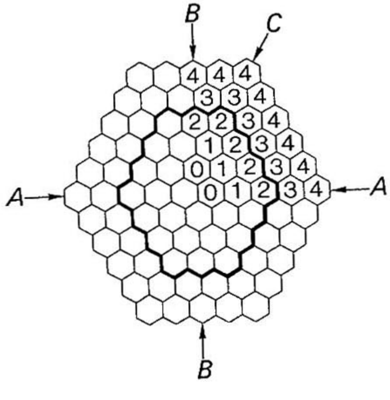

Fig. 3. Direct counting of distinct coronene hole positions in $(k+2)$–circumpyrenes. The inscribed numerals indicate k values.

Direct Combinatorics. The position of a coronene hole is determined uniquely by the central hexagon of coronene. Figure 3 illustrates a direct counting of the distinct positions of these holes. Because of symmetry only the hole centers in the segment $[A,B]$, viz. on and between the axes A and B should be counted (cf. Fig. 3). Let the numbers of isomers which belong to the symmetries [6] C_{2v}(a) or C_{2v}(b) be identified by the symbols M_k^{a} and M_k^{b}, respectively. They correspond to hole centers on the axis A or B, respectively. The U_k other isomers belong to C_s. The total number of isomers is given by

$$I_k = M_k^{\mathrm{a}} + M_k^{\mathrm{b}} + U_k \tag{5}$$

The direct counting of the numerals in Fig. 3 yields the differences:

k	0	1	2	3	4
ΔM_k^{a}	1	1	1	1	1
ΔM_k^{b}	1	0	1	0	1
ΔU_k	0	2	3	5	6
ΔI_k	2	3	5	6	8

For the absolute values these differences add up to:

k	0	1	2	3	4
M_k^{a}	1	2	3	4	5
M_k^{b}	1	1	2	2	3
U_k	0	2	5	10	16
I_k	2	5	10	16	24

In general, one finds easily the combinatorial expressions for the mirror-symmetrical (C_{2v}) systems:

$$M_k^{\mathrm{a}} = k + 1 \tag{6}$$

$$M_k^{\mathrm{b}} = \tfrac{k}{2} + 1 - \tfrac{1}{4}[1 - (-1)^k] = \lfloor k/2 \rfloor + 1 \tag{7}$$

For the unsymmetrical (C_s) systems, divide the numbers into U_k' and U_k'', pertaining to the sectors $\langle A,C\rangle$ (not including the axes) and $\langle B,C]$ (including C, but not B), respectively (cf. Fig. 3). Then one has for the differences:

k	0	1	2	3	4
$\Delta U_k'$	0	1	2	3	4
$\Delta U_k''$	0	1	1	2	2

In general, it is found:

$$\Delta U_k' = k \tag{8}$$

$$\Delta U_k'' = \frac{k}{2} + \frac{1}{4}[1 - (-1)^k] \tag{9}$$

Consequently,

$$\Delta U = \Delta U_k' + \Delta U_k'' = \frac{3k}{2} + \frac{1}{4}[1 - (-1)^k] \tag{10}$$

The expression for U_k is now deduced as:

$$U_k = \frac{3}{2}\sum_{i=0}^{k} i + \frac{1}{4}\sum_{i=0}^{k} [1 - (-1)^i] \tag{11}$$

where the last summation is

$$\sum_{i=0}^{k} [1 - (-1)^i] = k + \frac{1}{2}[1 - (-1)^k] \tag{12}$$

Consequently,

$$U_k = \frac{3}{2}\frac{k(k+1)}{2} + \frac{k}{4} + \frac{1}{8}[1 - (-1)^k] = \frac{1}{8}[6k^2 + 8k + 1 - (-1)^k] \tag{13}$$

On inserting from eqns. (6), (7) and (13) into (5) the following final expression was obtained.

$$I_k = \frac{1}{8}[6k^2 + 20k + 15 + (-1)^k] \tag{14}$$

The numerical values of U_k and I_k (see above) are seen to be shifted one place in the sense that

$$I_k = U_{k+1} \tag{15}$$

We can easily prove that this relation is valid in general. On substituting k by $(k+1)$ in eqn. (13) one indeed arrives at (14).

Combinatorics With Exploitation of Symmetry. It is clear from the above treatment that the numbers of the symmetrical isomers, viz. eqns. (6) and (7) were obtained considerably easier than those of the unsymmetrical isomers, viz. eqn. (13). In the following treatment the quantity U_k is eliminated. Start by counting the positions of coronene holes without regard to symmetry and call this "crude total" J_k. Then J_k is simply the number of hexagons in k–circumpyrene. It is obtained from eqn. (3) applied to the pyrene formula ($C_{16}H_{10}$) in combination with (1). This yields

$$J_k = 3k^2 + 7k + 4 = (k + 1)(3k + 4) \tag{16}$$

It is evident that J_k counts the symmetrical (C_{2v}) isomers twice and the unsymmetrical (C_s) four times. Hence

$$J_k = 2M_k^{\mathrm{a}} + 2M_k^{\mathrm{b}} + 4U_k \tag{17}$$

On eliminating U_k from eqns. (5) and (17) it is obtained

$$I_k = \frac{1}{4}(J_k + 2M_k^{\mathrm{a}} + 2M_k^{\mathrm{b}}) \tag{18}$$

The explicit expression for I_k is obtained on inserting into (18) the expressions from (6), (7) and (16). For the sake of variation, let us use the last (right–hand) expression for M_k^{b} from eqn. (7). Then the final result may be written

$$I_k = \frac{3}{4}(k + 1)(k + 2) + \frac{1}{2}(1 + \lfloor k/2 \rfloor) \tag{19}$$

which, of course, is equivalent to eqn. (14). Another alternative, which may be useful, reads:

$$I_k = \begin{cases} \frac{1}{4}(k + 2)(3k + 4); & k = 0, 2, 4, \ldots \\ \frac{1}{4}(k + 1)(3k + 7); & k = 1, 3, 7, \ldots \end{cases} \tag{20}$$

Generating Functions. Introduce:

$$M_{\mathrm{a}}(x) = \sum_{k=0}^{\infty} M_k^{\mathrm{a}} x^k = 1 + 2x + 3x^2 + 4x^3 + 5x^4 + \ldots \tag{21}$$

$$M_{\mathrm{b}}(x) = \sum_{k=0}^{\infty} M_k^{\mathrm{b}} x^k = 1 + x + 2x^2 + 2x^3 + 3x^4 + \ldots \tag{22}$$

$$I(x) = \sum_{k=0}^{\infty} I_k x^k = 2 + 5x + 10x^2 + 16x^3 + 24x^4 + \ldots \tag{23}$$

$$J(x) = \sum_{k=0}^{\infty} J_k x^k = 4 + 14x + 30x^2 + 52x^3 + 80x^4 + \ldots \tag{24}$$

An elementary result reads

$$\frac{1}{1-x} = 1 + x + x^2 + x^3 + x^4 + \ldots \tag{25}$$

In fact, this is already the generating function for ΔM_k^{a} (see above). The generating function for the absolute values from the differences is clearly obtained through division by $(1 - x)$; in this case:

$$\frac{1}{(1-x)^2} = 1 + 2x + 3x^2 + 4x^3 + 5x^4 + \ldots = \sum_{k=0}^{\infty} (k+1)x^k = M_{\mathrm{a}}(x) \tag{26}$$

In order to arrive at $M_{\mathrm{b}}(x)$, start from

$$\frac{1}{(1-x^2)^2} = 1 + 2x^2 + 3x^4 + 4x^6 + 5x^8 + \ldots \tag{27}$$

Consequently,

$$\frac{1+x}{(1-x^2)^2} = 1 + x + 2x^2 + 2x^3 + 3x^4 + \ldots = M_{\mathrm{b}}(x) = \frac{1}{(1-x)(1-x^2)} \tag{28}$$

The generating function for J_k is obtained most easily by means of

$$\frac{1}{(1-x)^3} = 1 + 3x + 6x^2 + 10x^3 + 15x^4 + \ldots = \sum_{k=0}^{\infty} \frac{(k+1)(k+2)}{2} x^k \tag{29}$$

Modify eqn. (16) to

$$J_k = 3(k+1)(k+2) - 2(k+1) \tag{30}$$

Then it is obtained, in accordance with eqns. (29) and (26):

$$J(x) = \frac{6}{(1-x)^3} - \frac{2}{(1-x)^2} = \frac{2(2+x)}{(1-x)^3} \tag{31}$$

The relation (18) is valid for the corresponding generating functions; in other words:

$$I(x) = \frac{1}{4}[J(x) + 2M_a(x) + 2M_b(x)] \tag{32}$$

Now, on inserting the expressions from (26), (28) and (31) one obtains the explicit form of $I(x)$ as

$$I(x) = \frac{2+x}{(1-x)^2(1-x^2)} \tag{33}$$

The last step may be facilitated by virtue of eqn. (15). When translated to generating functions it reads

$$U(x) = x\, I(x) \tag{34}$$

where

$$U(x) = \sum_{k=0}^{\infty} U_k x^k = 2x + 5x^2 + 10x^3 + 16x^4 + \ldots \tag{35}$$

In analogy with eqn. (5) one has

$$I(x) = M_a(x) + M_b(x) + U(x) \tag{36}$$

which on combining with (34) yields

$$I(x) = \frac{1}{1-x}[M_a(x) + M_b(x)] \tag{37}$$

The result for $I(x)$ as in (33) is readily reproduced on inserting the expressions from (26) and (28) into (37).

Extension to All Coronenic Perforated Circular Benzenoids. For the sake of brevity we shall not report the details in the following analysis. Let C_nH_s be the formula of one of the title systems for $k = 0$. Six representatives for the six different ϵ values are depicted in Fig. 2. For the crude total (J_k) the following general expression was found.

$$J_k = 3k^2 + k(s - 21) + \frac{1}{2}(n - 5s) + 37 \tag{38}$$

Eqn. (16) is the special case for $C_{16}H_{10}$. The generating function for J_k was determined as:

$$J(x) = \frac{n-5s+74+2x(6s-n-92)+x^2(n-7s+122)}{2(1-x)^3} \tag{39}$$

Eqn. (31) is the special case for $C_{16}H_{10}$. The generalizations of eqns. (19) and (33) for the total numbers of isomers in the forms I_k and $I(x)$, respectively, are collected in Table 1.

The numerical results of I_k for $k \leq 6$ are shown in Table 2. For the corresponding C_nH_s formulas, Table 3 may be consulted.

Table 1. Numbers of isomers of coronenic perforated circular benzenoids: explicit formulas I_k; generating functions $I(x)$.

ϵ	I_k	$I(x)$
0	$\frac{1}{12}(3k^2+9k+12+6\lfloor k/2 \rfloor)$	$(1-x)^{-2}(1-x^2)^{-1}$
1	$\frac{1}{2}(3k^2+5k+2)$	$(1+2x)(1-x)^{-3}$
2	$\frac{1}{4}(3k^2+7k+4+2\lceil k/2 \rceil)$	$(1+2x)(1-x)^{-2}(1-x^2)^{-1}$
3	$\frac{1}{2}(k^2+3k+2)=\binom{k+2}{2}$	$(1-x)^{-3}$
4	$\frac{1}{4}(3k^2+9k+8+2\lfloor k/2 \rfloor)$	$(2+x)(1-x)^{-2}(1-x^2)^{-1}$
5	$\frac{3}{2}(k^2+3k+2)=3\binom{k+2}{2}$	$3(1-x)^{-3}$

Table 2. Numbers of isomers of coronenic perforated circular coronoids. For the C_nH_s formulas, see Table 3.

	ϵ					
k	0	1	2	3	4	5
0	1	1	1	1	2	3
1	2	5	4	3	5	9
2	4	12	8	6	10	18
3	6	22	14	10	16	30
4	9	35	21	15	24	45
5	12	51	30	21	33	63
6	16	70	40	28	44	84

Table 3. Formulas of coronenic perforated circular benzenoids.

k	ϵ 0	1	2	3	4	5
0	$C_{48}H_{24}$	$C_{53}H_{25}$	$C_{60}H_{26}$	$C_{67}H_{27}$	$C_{74}H_{28}$	$C_{81}H_{29}$
1	$C_{90}H_{30}$	$C_{97}H_{31}$	$C_{106}H_{32}$	$C_{115}H_{33}$	$C_{124}H_{34}$	$C_{133}H_{35}$
2	$C_{144}H_{36}$	$C_{153}H_{37}$	$C_{164}H_{38}$	$C_{175}H_{39}$	$C_{186}H_{40}$	$C_{197}H_{41}$
3	$C_{210}H_{42}$	$C_{221}H_{43}$	$C_{234}H_{44}$	$C_{247}H_{45}$	$C_{260}H_{46}$	$C_{273}H_{47}$
4	$C_{288}H_{48}$	$C_{301}H_{49}$	$C_{316}H_{50}$	$C_{331}H_{51}$	$C_{346}H_{52}$	$C_{361}H_{53}$
5	$C_{378}H_{54}$	$C_{393}H_{55}$	$C_{410}H_{56}$	$C_{427}H_{57}$	$C_{444}H_{58}$	$C_{461}H_{59}$
6	$C_{480}H_{60}$	$C_{497}H_{61}$	$C_{516}H_{62}$	$C_{535}H_{63}$	$C_{554}H_{64}$	$C_{573}H_{65}$

General Formulations. General expressions for formula sequences similar to that of Table 3 (viz. $C_{48}H_{24}$, $C_{53}H_{25}$, $C_{60}H_{26}$, ...) have been developed in the theory of benzenoids [9,10]. Two different approaches are employed therein and referred to as the "Harary–Harborth picture" and the "Balaban picture". These designations are rational since the treatments are based on an analysis of Harary and Harborth [19] in the former case, while it is closely related to Balaban [20] in the latter. Here we are able to extend the list by a new "picture" in terms of a generating function. No details of the derivation are given for the sake of brevity.

Harary–Harborth Picture. The formulas $C_nH_s \equiv (n;s)$ of C, the coronenic perforated circular benzenoids (cf. Table 3) are considered.

$$(n;s) = (2\lfloor\tfrac{1}{12}(s^2-6s)\rfloor - s;\ s) \qquad (40)$$

where $s = 24, 25, 26, \ldots$.

Balaban Picture. The formula $(n;s)$ of C is determined by the two parameters ϵ and k.

$$(n;s) = (6(k+2)(k+4) + (2k+7)\epsilon - 2\lceil\epsilon/6\rceil;\ 6k + 24 + \epsilon) \qquad (41)$$

where $k = 0, 1, 2, \ldots$, and $\epsilon = 0, 1, 2, 3, 4, 5$.

New Picture. Let the generating function for the coefficients n of C_nH_s for C be defined by

$$n(x) = \sum_{s=24}^{\infty} n_s x^s = 48x^{24} + 53x^{25} + 60x^{26} + 67x^{27} + 74x^{28} + \ldots \qquad (42)$$

Then an explicit form of $n(x)$ reads:

$$n(x) = \frac{x^{24}(48+5x+7x^2+7x^3+7x^4+7x^5-87x^6-3x^7-5x^8-5x^9-5x^{10}-5x^{11}+41x^{12})}{(1-x)(1-x^6)^2} \qquad (43)$$

Conclusion. The enumeration methods, which were applied in the present work, are altogether not new. Generating functions in particular have been employed many times [21–28]. Also the symmetry has been exploited to a large extent [21–25,27,29–34]. In this connection the work by Redelmeier [33] is especially relevant. On the other hand, the applications of these enumeration methods are new. It is not claimed, however, that these applications in themselves have much interest for chemists. That was not the main intention of this work, but as the title suggests, this is mainly intended to be a demonstration of the methods as a "course in enumeration", using the special systems (coronoids) as an example. Elementary for mathematicians, useful for chemists.

Under this scope it is believed that this exposition preserves some of the good traditions from the late Professor O. E. Polansky, founder of Match. We have cited a paper by Polansky and Rouvray [18] in the above text. It represents the first paper of a short series [18,35–38], which can be characterized (more or less) as educational. Polansky has also proved his eminent pedagogical abilities in other publications [39,40].

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The "Computer Corner" of this issue announces a computer program for special generating functions. It applies to all the generating functions encountered in the present article.