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NUMBER OF KEKULÉ STRUCTURES FOR RECTANGLE-SHAPED BENZENOIDS

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Abstract - The number of Kekulé structures (K) of oblate rectangular benzenoids (with indentation outwards) are studied. Rj(m,n) is used to denote the oblate rectangle with $2m-1$ tier chains of alternating lengths n and $n+1$ (in terms of the number of hexagons). The previous results are extended by algebraic combinatorial formulas for the K numbers of Rj$(m,3)$ and Rj$(4,n)$. In order to reach the latter goal the enumeration problem for 9 additional benzenoid classes had to be solved. New variants of the enumeration techniques are employed and seem to deserve the status of new methods. A fully computerized method was also developed; it leads to an equivalent algebraic formula for $K\{\mathrm{Rj}(4,n)\}$.

1. INTRODUCTION

The enumeration of Kekulé structures of benzenoid systems has attracted many investigators. Peri-condensed benzenoids in the shapes of a parallelogram, hexagon, zig-zag chain or a rectangle are very regular and recognized as important classes [1, 2]. Combinatorial algebraic formulas have been produced for the general case of a parallelogram in the classical work of Gordon and Davison [1], who also reported the formulas for hexagons with at least four sides equal. The general case of hexagons was solved more recently by Cyvin [3]. The zig-zag chains were studied most extensively by Gutman and Cyvin [4]. They reported combinatorial formulas for n-tuple zig-zag chains with m up to 8, each expression being a polynomial of m-th degree in n. The enumeration of Kekulé structures of rectangle-shaped benzenoids is the topic of the present work.

2. DEFINITIONS

A rectangle-shaped benzenoid or simply rectangle has both "vertical" sides indented. It is important to distinguish between prolate and oblate

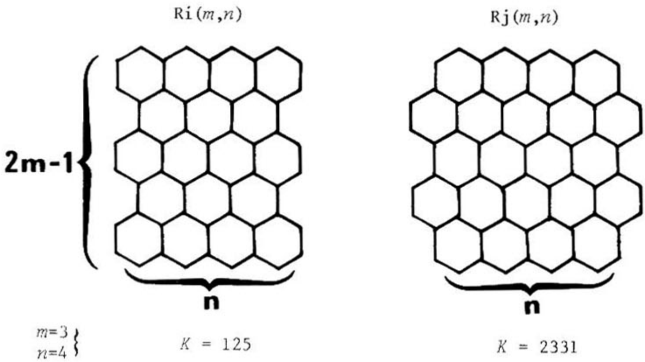


Fig. 1. Definition of the prolate (Ri) and oblate (Rj) rectangle.

rectangles [5], with inwards and outwards indentation, respectively; they are denoted Ri (inwards) and Rj (outwards). The system of indices (cf. Fig. 1) is adopted from Yen [2].

This researcher [2] was also the first one to give the general formula of the number of Kekulé structures (K) of a prolate reclangle, viz. $(n+1)^m$. In the following only the oblate rectangles are treated.

3. SUMMARY OF RESULTS

3.1. *Oblate rectangles with fixed values of n*

Gutman [6] produced the combinatorial formulas for K numbers of Rj(m,1) and Rj(m,2); see CHART I. In the present work the analysis was extended to Rj(m,3). These formulas were derived from recurrence relations. Such a relation is also given here for Rj(m,4). The recurrence formulas were used to compute some of the numerical values in TABLE 1.

3.2. *Oblate rectangles with fixed values of m*

The combinatorial formulas of K for the 3-tier (m=2) [1] and 5-tier (m=3) [1, 2, 7] oblate rectangles are long known; cf. CHART II. The chart includes the present result for m=4, the corresponding 7-tier strip.

3.3. *Numerical results*

TABLE 1 shows the numerical values of K numbers for some oblate rectangles with $n \leq 10$ and $m \leq 10$. They were determined by means of the appropriate algebraic formulas along with some supplementary numerical computations (see below). Some of the values were checked directly by means of a general computer-program for K numbers.

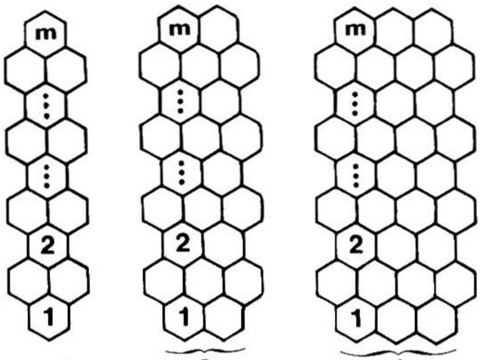
4. AUXILIARY BENZENOID CLASSES

The utility of auxiliary benzenoid classes was demonstrated by Gutman [6] and later by Gutman and Cyvin [4]. Such classes also play an important role in the present work. In Fig. 2 four auxiliary classes are depicted. Only for the simplest one the explicit algebraic formula of the K numbers is known [5], viz.

$$K\{B(n,2,-l)\} = \binom{n+2}{2}(l+1) - (n+2)\binom{l+1}{2} \tag{1}$$

CHART I - Three oblate rectangular benzenoids (fixed n)

Rj$(m,1)$ Rj$(m,2)$ Rj$(m,3)$



$m \geq 1$ 2 3

[a] $K\{\mathrm{Rj}(m,1)\} = 2 \cdot 3^{m-1}$

[a] $K\{\mathrm{Rj}(m,2)\} = \frac{1}{16}\left[(4+\sqrt{8})^{m+1} + (4-\sqrt{8})^{m+1}\right]$

$K\{\mathrm{Rj}(m,3)\}$

$$= \frac{2}{\sqrt{5}}\left\{(\sqrt{5}+2)\left[\frac{5}{2}(3+\sqrt{5})\right]^{m-1} + (\sqrt{5}-2)\left[\frac{5}{2}(3-\sqrt{5})\right]^{m-1}\right\}$$

[a] I. Gutman, Match 17, 3 (1985).

TABLE 1. Numerical values of $K\{\mathrm{Rj}(m,n)\}$.*

m \ n	1	2	3	4	5	6	7	8	9	10
1	2	3	4	5	6	7	8	9	10	11
2	6	20	50	105	196	336	540	825	1210	1716
3	18	136	650	2331	6860	17472	39852	83325	162382	298584
4	54	928	8500	52137	242158	916992	2969946	8501625		
5	162	6336	111250	1167291	8557164					
6	486	43264	1456250							
7	1458	295424								
8	4374	2017280								
9	13122									
10	39366									

*Values greater than 10^7 are not entered

Rj(m,n)

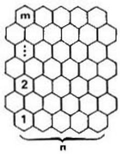
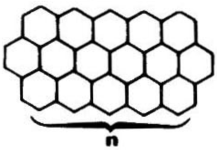
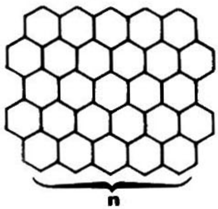


CHART II - Three oblate rectangular benzenoids (fixed m)

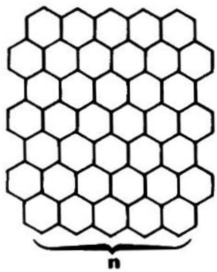
Rj$(2,n)$



Rj$(3,n)$



Rj$(4,n)$



[a] $K\{\mathrm{Rj}(2,n)\}$

$$= \frac{1}{12}(n+1)(n+2)^2(n+3)$$

[a–c] $$K\{\mathrm{Rj}(3,n)\} = \frac{1}{120}(n+1)(n+2)^3(n+3)(n^2 + 4n + 5)$$

$$K\{\mathrm{Rj}(4,n)\} = \frac{1}{20160}(n+1)(n+2)^4(n+3)(17n^4 + 136n^3 + 439n^2 + 668n + 420)$$

[a]M. Gordon and W.H.T. Davison, J. Chem. Phys. 20, 428 (1952).

[b]T.F. Yen, Theoret. Chim. Acta 20, 399 (1971).

[c]N. Ohkami and H. Hosoya, Theoret. Chim. Acta 64, 153 (1983).

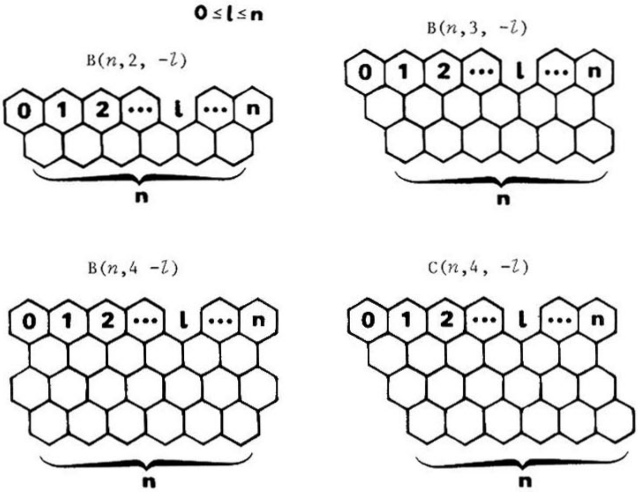


Fig. 2. Four auxiliary benzenoid classes.

5. OBLATE RECTANGLES WITH FIXED VALUES OF n

5.1. *The case of* n=3

Gutman's method [6] was applied to the case of $\mathrm{Rj}(m,3)$. In this case we need the benzenoid classes $B(3,\ 2m-2,\ l)$, where l = -1, 0, 1 and 2. The definition for the negative value of l should be clear from Fig. 2, where the second index in B may be extended to 6, 8, 10, ... in an obvious way. The definition for positive values of l is explained in Fig. 3, which also includes l=0; the latter case coincides with the definition for $l \leq 0$. In this notation $B(3,\ 2m-2,\ 3) = \mathrm{Rj}(m,3)$. Introduce also the symbol $K_l(m')$ to identify the number of Kekulé structures for $B(3,\ 2m',\ l)$, where $m' = m-1$. The following equations (for $m' \geq 1$) were found, all in terms of $K_3(m')$ and $K_3(m'-1)$, which are K numbers for oblate rectangles.

$$K_2(m') = K_3(m') - \frac{5}{2} K_3(m'-1)$$
$$K_1(m') = \frac{1}{2} K_3(m')$$
$$K_0(m') = \frac{5}{2} K_3(m'-1)$$
$$K_{-1}(m') = \frac{1}{2} K_3(m') - \frac{5}{2} K_3(m'-1)$$

Furthermore it was arrived at the recurrence formula

$$K_3(m') = 5[3K_3(m'-1) - 5K_3(m'-2)]; \qquad m' \geq 2$$

This relation is equivalent to

$$K\{\mathrm{Rj}(m,3)\} = 15K\{\mathrm{Rj}(m-1, 3)\} - 25K\{\mathrm{Rj}(m-2, 3)\}; \qquad m \geq 3 \qquad (2)$$

Along with the initial conditions $K\{\mathrm{Rj}(1,3)\} = 4$ (anthracene) and $K\{\mathrm{Rj}(2,3)\} = 50$ (ovalene) it determines all K numbers for $\mathrm{Rj}(m,3)$ with arbitrary m values. The derived explicit formula is shown in CHART I.

5.2. *The case of* $n=4$

A recurrence formula was also derived for $\mathrm{Rj}(m,4)$. In this case let $K_l(m')$ denote the K numbers for $\mathrm{B}(4, 2m', l)$, where $l = -2, -1, 0, 1, 2, 3$ and 4; $m' = m-1$. Consequently $K_4(m') = K\{\mathrm{Rj}(m,4)\}$. In this case it was found ($m' \geq 2$):

$$K_3(m') = K_4(m') - 3K_4(m'-1)$$

$$K_2(m') = K_4(m') - 9K_k(m'-1) + 18K_4(m'-2)$$

$$K_1(m') = 9K_4(m'-1) - 18K_4(m'-2)$$

$$K_0(m') = 3K_4(m'-1)$$

$$K_{-1}(m') = 6K_4(m'-1) - 18K_4(m'-2)$$

$$K_{-2}(m') = K_4(m') - 18K_4(m'-1) + 36K_4(m'-2)$$

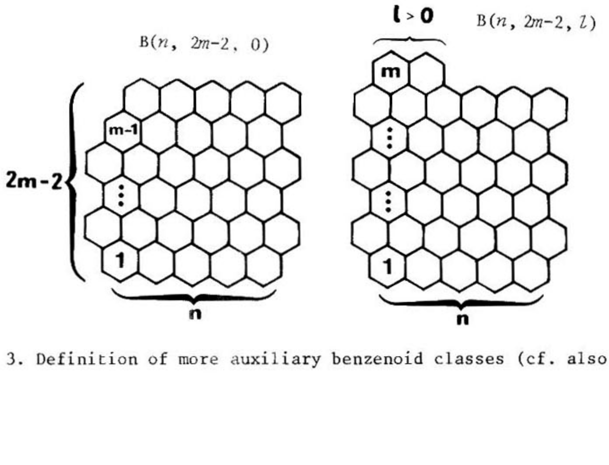


Fig. 3. Definition of more auxiliary benzenoid classes (cf. also Fig. 2).

Finally it was arrived at the recurrence formula

$$K_4(m') = 27[K_4(m'-1) - 4K_4(m'-2) + 4K_4(m'-3)]; \qquad m' \geq 3$$

which is equivalent to:

$$K\{\mathrm{Rj}(m,4)\} = 27K\{\mathrm{Rj}(m-1,\ 4)\} - 108K\{\mathrm{Rj}(m-2,\ 4)\} + 108K\{\mathrm{Rj}(m-3,\ 4)\}; \qquad m \geq 4 \tag{3}$$

In order to determine the K numbers for arbitrary values of m we also need the initial conditions $K\{\mathrm{Rj}(m,4)\} = 5$, 105 and 2331 for $m = 1$, 2 and 3, respectively.

6. BASIC FORMULAS

We now turn to the enumeration of Kekulé structures for the 7-tier oblate rectangles, $\mathrm{Rj}(4,n)$ with arbitrary values of n; cf. CHART II. None of the previously applied methods for the corresponding 5-tier strip [1, 2, 7] seem to be amenable for a generalization to higher rectangles. The present result of $K\{\mathrm{Rj}(4,n)\}$ (cf. CHART II) was achieved by refined applications of the auxiliary benzenoid classes shown in Fig. 2. New variants of the enumeration techniques had to be employed, and a number of benzenoid classes of 5-tier, 6-tier and 7-tier strips had to be solved before the goal was reached.

A basic formula, viz.

$$K\{\mathrm{Rj}(4,n)\} = \sum_{i=0}^{n} K\{\mathrm{B}(n,4,\ -i)\}\cdot K\{\mathrm{B}(n,2,\ -i)\} \tag{4}$$

is obtained by means of the well-known [8] enumeration techniques of fragmentation, which is supposed to be applied n times; cf. Fig. 4. The thick arrows point out the bonds which are attacked each time. In this process one arrives at a series of essentially disconnected benzenoids, for which the total K number is equal to the product of K numbers of the two parts.

The type of formula (4) is quite general for oblate rectangles. One has actually

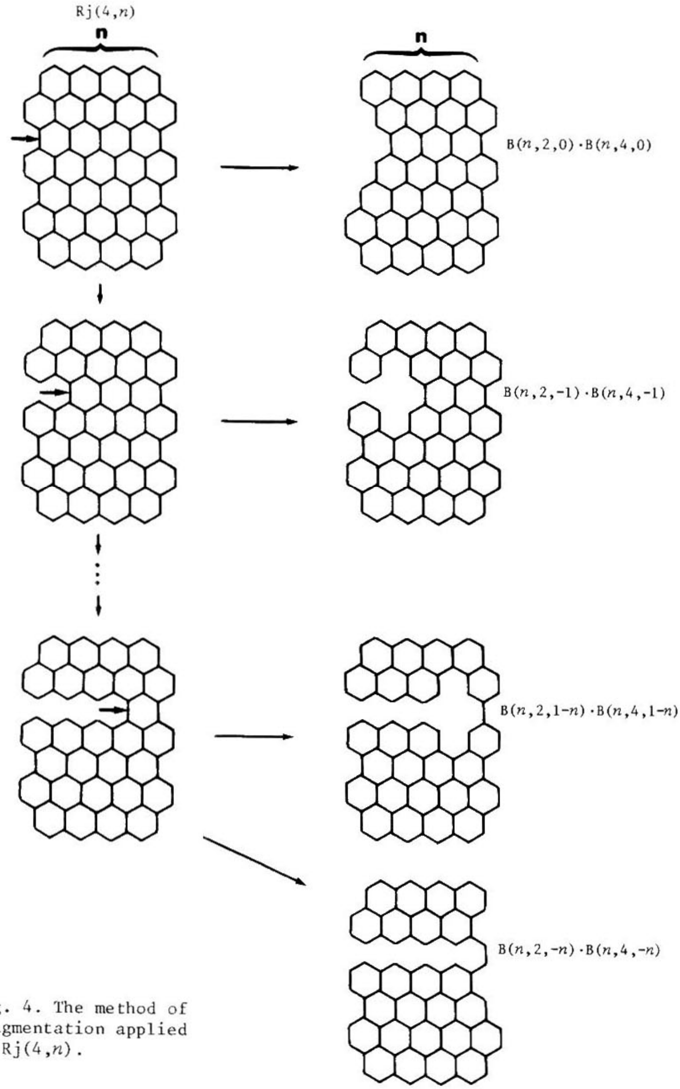


Fig. 4. The method of fragmentation applied to Rj(4,n).

$$K\{\mathrm{Rj}(m,n)\} = \sum_{i=0}^{n} K\{\mathrm{B}(n,\ 2m-2,\ -i)\}$$

$$= \sum_{i=0}^{n} K\{\mathrm{B}(n,\ 2p,\ -i)\}\cdot K\{\mathrm{B}(n,\ 2q,\ -i)\} \qquad (5)$$

where p and q (positive integers) fulfil the condition $p+q = m-1$. Thus, for instance, for the 9-tier oblate rectangle:

$$K\{\mathrm{Rj}(5,n)\} = \sum_{i=0}^{n} K\{\mathrm{B}(n,8,\ -i)\} = \sum_{i=0}^{n} K\{\mathrm{B}(n,6,\ -i)\}\cdot K\{\mathrm{B}(n,2,\ -i)\}$$

$$= \sum_{i=0}^{n} [K\{\mathrm{B}(n,4,\ -i)\}]^2 \qquad (6)$$

The numbers $K\{\mathrm{B}(n,4,\ -l)\}$ were computed numerically for some values of n and l. TABLE 2 shows, as an example, the results for $n=5$. Also included are the corresponding numerical values for $K\{\mathrm{B}(n,2,\ -l)\}$, which conform with eqn. (1). With reference to the notation in TABLE 2 one obtains (cf. TABLE 1):

TABLE 2. Numerical values of $x_l = K\{\mathrm{B}(5,2,\ -l)\}$ and $y_l = K\{\mathrm{B}(5,4,\ -l)\}$.

l	x	y
0	21	686
1	35	1225
2	42	1519
3	42	1519
4	35	1225
5	21	686

$$K\{\mathrm{R}(2,5)\} = \sum_{i=0}^{5} x_i = 196$$

$$K\{\mathrm{R}(3,5)\} = \sum_{i=0}^{5} y_i = \sum_{i=0}^{5} x_i^2 = 6860$$

$$K\{\mathrm{R}(4,5)\} = \sum_{i=0}^{5} x_i y_i = 242158$$

$$K\{\mathrm{R}(5,5)\} = \sum_{i=0}^{5} y_i^2 = 8557164$$

Now we turn back to the algebraic solution of eqn. (4). The idea is to achieve this goal without having an algebraic solution for the auxiliary benzenoids $B(n,4,\ -i)$. On inserting the expression for $B(n,2,\ -i)$ from eqn. (1) into (4) one attains at

$$K\{Rj(4,n)\} = \binom{n+3}{2}\sum_{i=0}^{n} K\{B(n,4,\ -i)\}(i+1) - (n+2)\sum_{i=0}^{n} K\{B(n,4,\ -i)\}\binom{i+2}{2}$$

$$= \binom{n+3}{2}\sum_{i=0}^{n} K\{B(n,4,\ -i)\}\cdot K\{L(i)\} - (n+2)\sum_{i=0}^{n} K\{B(n,4,\ -i)\}\cdot K\{L(2,i)\} \qquad (7)$$

Here $L(i)$ and $L(2,i)$ are well-known benzenoids, viz. the linear single chain and 2-tier parallelogram [1]. The two summations of eqn. (7) are identified with the K numbers of certain benzenoid classes, viz.

$$K\{Rj(4,n)\} = \binom{n+3}{2} K\{H(3,4,n)\} - (n+2)\ K\{H(3,5,n)\} \qquad (8)$$

The two types of benzenoids are depicted in Fig. 5. The indices $(3,4,n)$ and $(3,5,n)$ are used because they refer to sub-benzenoids of the hexagon-shaped classes [3] $O(3,4,n)$ and $O(3,5,n)$, respectively. The identity with the summations of eqn. (7) become apparent when the benzenoids are treated by the method of fragmentation according to the same pattern as applied to $Rj(4,n)$; it is illustrated in Fig. 4. Figure 5 indicates by arrows marked r the first bonds to be attacked in this procedure.

Before we start to enumerate the Kekulé structures of the two benzenoid classes of Fig. 5 we will solve some simpler problems, which will prove to be useful in the following.

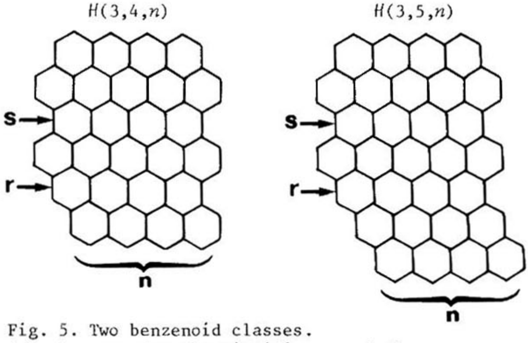
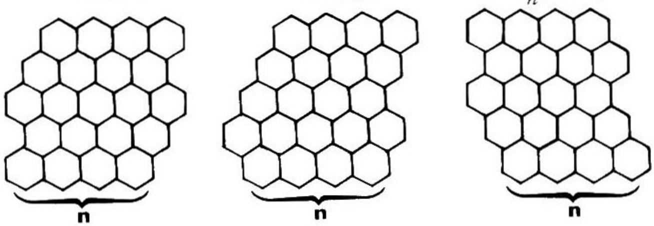


Fig. 5. Two benzenoid classes.
See the text for the significance of the arrows.

CHART III - Three 5-tier strips

Ob$(2,4,n)$ Di$(2,4,n)$ $\mathrm{M}_n(L^2A^2L)$



$$K\{\mathrm{Ob}(2,4,n)\} = \frac{1}{360}(n+1)(n+2)^2(n+3)(7n^2 + 28n + 30)$$

$$K\{\mathrm{Di}(2,4,n)\} = \frac{1}{240}(n+1)(n+2)^2(n+3)(n+4)(3n + 5)$$

$$K\{\mathrm{M}_n(L^2A^2L)\} = \frac{1}{120}(n+1)(n+2)(n+3)(9n^2 + 26n + 20)$$

7. THREE FIVE-TIER STRIPS

7.1. *Introduction*

CHART III shows three benzenoid classes of 5-tier strips, all of them sub-benzenoids of the hexagon O$(2,4,n)$. Here $\mathrm{M}_n(L^2A^2L)$ or $\mathrm{M}_n(LLAAL)$ is a multiple chain, where the parenthesized symbols refer to the LA-sequence[9].

7.2. *The class* Ob$(2,4,n)$

The benzenoid Ob$(2,4,n)$ is actually a hexagon without two corners, to which Cyvin's theory [3] is applicable. One obtains

$$K\{\mathrm{Ob}(2,4,n)\} = K\{\mathrm{O}(2,n,4)\} - 2K\{\mathrm{O}(2,\ n-1,\ 4)\} + K\{\mathrm{O}(2,\ n-2,\ 4)\}$$

$$= \frac{1}{5}\binom{n+4}{4}\binom{n+5}{4} - \frac{2}{5}\binom{n+3}{4}\binom{n+4}{4} + \frac{1}{5}\binom{n+2}{4}\binom{n+3}{4} \qquad (9)$$

This expression was worked out to yield the polynomial-form in CHART III.

7.3. *The n-tuple chain* $\mathrm{M}_n(L^2A^2L)$

The method of fragmentation [8] was applied to $\mathrm{M}_n(L^2A^2L)$ according to

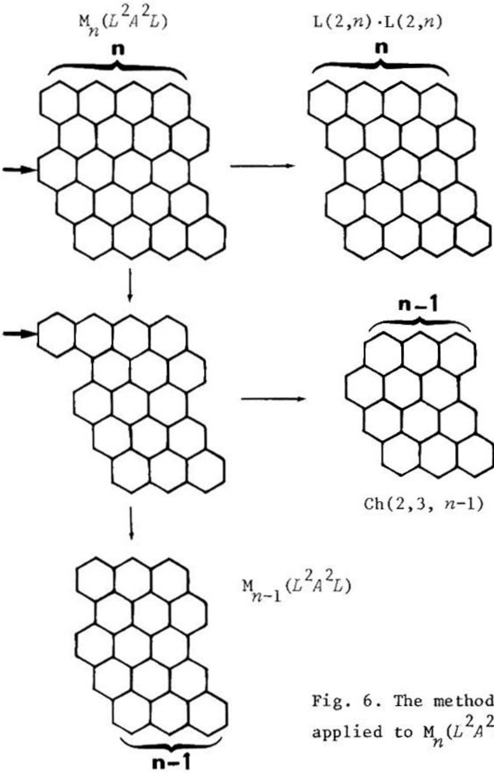


Fig. 6. The method of fragmentation applied to $M_n(L^2A^2L)$.

Fig. 6. Thereby it was achieved to arrive at $M_{n-1}(L^2A^2L)$ as one of the fragments. Hence one attains at a recurrence formula:

$$K\{M_n(L^2A^2L)\} - K\{M_{n-1}(L^2A^2L)\} = [K\{L(2,n)\}]^2 + K\{Ch(2,2,\ n-1)\}; \quad n \geq 1 \tag{10}$$

The required formulas of K numbers on the right-hand side of this equation are known. In particular is the symbol Ch used to denote a chevron-shaped benzenoid [10]. In total one obtains

$$K\{M_n(L^2A^2L)\} - K\{M_{n-1}(L^2A^2L)\} = \binom{n+2}{2}^2 + n\binom{n+2}{3} - \binom{n+2}{4} \tag{11}$$

With the initial condition $K\{\mathrm{M}_0(L^2A^2L)\} = 1$ one attains at the summation formula

$$K\{\mathrm{M}_n(L^2A^2L)\} = \sum_{i=0}^{n} \binom{i+2}{2}^2 + \sum_{i=1}^{n} i \binom{i+2}{3} - \sum_{i=2}^{n} \binom{i+2}{4} \tag{12}$$

The summations were worked out to yield

$$K\{\mathrm{M}_n(L^2A^2L)\} = \binom{n+2}{2}\binom{n+3}{3} - \binom{n+4}{5} \tag{13}$$

or the polynomial-form quoted in CHART III.

7.4. *The class* Di$(2,4,n)$

The members of the class Di$(2,4,n)$ may be referred to as prolate pentagons; cf. CHART III. The method of fragmentation (cf. Fig. 7) gives the recurrence formula

$$K\{\mathrm{Di}(2,4,n)\} - K\{\mathrm{Di}(2,4,\ n-1)\} = K\{\mathrm{M}_n(L^2A^2L)\} = \binom{n+2}{2}\binom{n+3}{3} - \binom{n+4}{5} \tag{14}$$

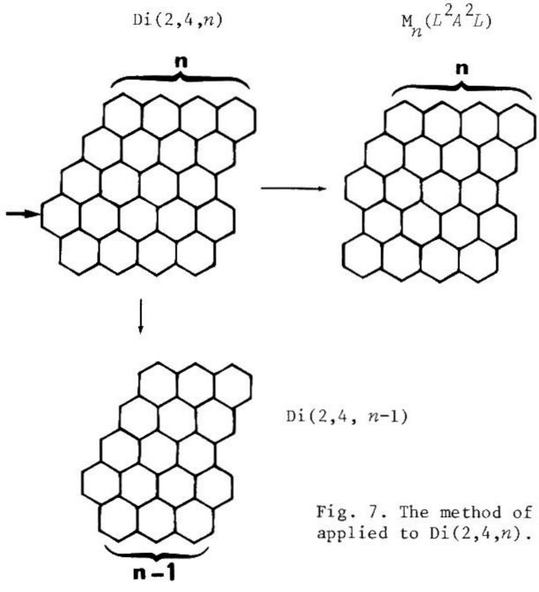


Fig. 7. The method of fragmentation applied to Di$(2,4,n)$.

where the expression from eqn. (13) is inserted. This leads to the summation formula

$$K\{\mathrm{Di}(2,4,n)\} = \sum_{i=0}^{n} \binom{i+2}{2}\binom{i+3}{3} - \sum_{i=1}^{n} \binom{i+4}{5} \tag{15}$$

The summations were worked out to yield the result quoted in CHART III.

8. THREE SIX-TIER STRIPS

8.1. *Basic formula*

According to eqn. (8) we are primarily interested in $H(3,4,n)$ among the 6-tier strips; cf. Fig. 5. We will use the refined application of auxiliary classes described in Section 6. When the method of fragmentation is applied with respect to the bond marked s in Fig. 5 one realizes

$$K\{H(3,4,n)\} = \sum_{i=0}^{n} K\{\mathrm{B}(n,3,\ -i)\}\cdot K\{\mathrm{B}(n,2,\ -i)\}$$

$$= \binom{n+3}{2} \sum_{i=0}^{n} K\{\mathrm{B}(n,3,\ -i)\}\cdot K\{\mathrm{L}(i)\} - (n+2) \sum_{i=0}^{n} K\{\mathrm{B}(n,3,\ -i)\}\cdot K\{\mathrm{L}(2,i)\} \tag{16}$$

Here again the two summations on the right-hand side are identified with the K numbers of certain benzenoids;

$$K\{H(3,4,n)\} = \binom{n+3}{2} K\{\mathrm{Ob}(2,4,n)\} - (n+2)K\{H(2,5,n)\} \tag{17}$$

The K formula of $\mathrm{Ob}(2,4,n)$ was found in Section 7.2. In order to solve this problem for the benzenoids referred to as $H(2,5,n)$ we have first attacked the multiple chain of $\mathrm{M}_n(L^3A^2L)$. Both these classes are sub-benzenoids of $\mathrm{O}(2,5,n)$; cf. CHART IV.

8.2. *The n-tuple chain* $\mathrm{M}_n(L^3A^2L)$

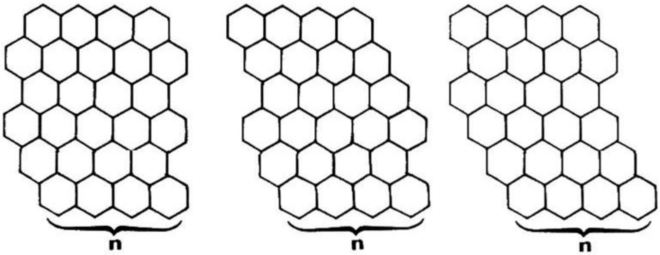
The method applied in Section 7.3 (cf. also Fig. 6) may be generalized straightforwardly to the case of $\mathrm{M}_n(L^pA^2L)$, where p is a positive integer. The result is

$$K\{\mathrm{M}_n(L^pA^2L)\} = \binom{n+2}{2}\binom{n+p+1}{p+1} - \binom{n+p+2}{p+3} \tag{18}$$

Equation (13) is the special case of p=2. With p=3 one attains at an

CHART IV - Three 6-tier strips

$H(3,4,n)$ $\quad$ $H(2,5,n)$ $\quad$ $M_n(L^3A^2L)$



$$K\{H(3,4,n)\} = \frac{1}{240}(n+1)(n+2)^4(n+3)(n^2 + 4n + 5)$$

$$K\{H(2,5,n)\} = \frac{1}{720}(n+1)(n+2)^2(n+3)(4n^3 + 31n^2 + 75n + 60)$$

$$K\{M_n(L^3A^2L)\} = \frac{1}{360}(n+1)(n+2)(n+3)(n+4)(7n^2 + 20n + 15)$$

expression which is equivalent to the polynomial-form in CHART IV.

8.3. *The class* $H(2,5,n)$

A benzenoid belonging to $H(2,5,n)$ is depicted in CHART IV. The method of fragmentation was applied in a similar way as in Sections 7.3 and 7.4, but in three steps. Also in this case a recurrence formula was achieved:

$$K\{H(2,5,n)\} - K\{H(2,5,\ n-1)\}$$

$$= K\{M_n(L^3A^2L)\} + K\{Ob(2,4,\ n-1)\} + K\{D(2,3,\ n-1)\}; \qquad n \geq 1 \qquad (19)$$

Here the desired K formula for $M_n(L^3A^2L)$ was found in Section 8.2 (cf. also CHART IV) and the one of $Ob(2,4,n)$ in Section 7.2 (cf. also CHART III). The remaining K number pertains to the 4-tier pentagon, for which the formula is known [3]:

$$K\{D(2,3,n)\} = \frac{1}{4}(n+2)^2 \binom{n+3}{3} \qquad (20)$$

On inserting the appropriate formulas (two of them with n substituted by n-1) into eqn. (19) one attains at

$$K\{H(2,5,n)\} - K\{H(2,5,\ n-1)\} = \frac{1}{60}\binom{n+3}{3}(2n+3)(7n^2+21n+20) \qquad (21)$$

This leads to the summation formula

$$K\{H(2,5,n)\} = \frac{1}{60}\sum_{i=0}^{n}\binom{i+3}{3}(2i+3)(7i^2+21i+20) \qquad (22)$$

This sum was worked out into the expression of CHART IV.

8.4. *The class* $H(3,4,n)$

The desired K formulas to be inserted into eqn. (17) have now been determined (cf. CHARTS III and IV). Consequently we arrive at the formula for $H(3,4,n)$. It is included in CHART IV.

9. THREE SEVEN-TIER STRIPS

9.1. *Basic formula*

We are primarily interested in $H(3,5,n)$; cf. again eqn. (8). A partitioning similar to eqn. (16) of Section 8.1 reads

$$K\{H(3,5,n)\} = \sum_{i=0}^{n} K\{\mathrm{C}(n,4,\ -i)\}\cdot K\{\mathrm{B}(n,2,\ -i)\}$$

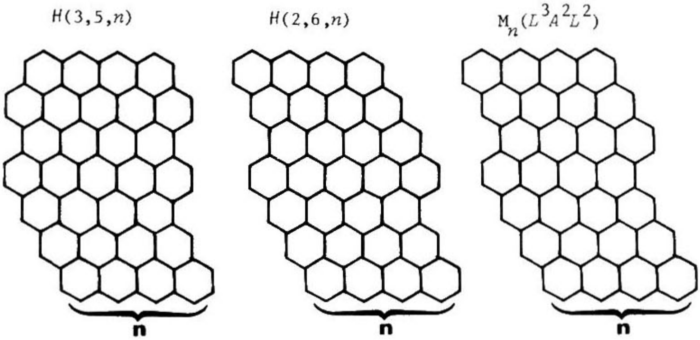
$$= \binom{n+3}{2}\sum_{i=0}^{n} K\{\mathrm{C}(n,4,\ -i)\}\cdot K\{\mathrm{L}(i)\} - (n+2)\sum_{i=0}^{n} K\{\mathrm{C}(n,4,\ -i)\}\cdot K\{\mathrm{L}(2,i)\} \qquad (23)$$

This result was again obtained by the method of fragmentation when focusing the attention on the arrow marked s in Fig. 5. The two summations on the right-hand side are identified with K numbers of certain benzenoids according to:

$$K\{H(3,5,n)\} = \binom{n+3}{2} K\{H(2,5,n)\} - (n+2)K\{H(2,6,n)\} \qquad (24)$$

The K formula for $H(2,5,n)$ was found in Section 8.3. The benzenoid $H(2,6,n)$ is depicted in CHART V and treated in a subsequent section. But first we need to find the K formula for the multiple chain also shown in CHART V. The two latter benzenoids are both sub-benzenoids of $O(2,6,n)$.

CHART V - Three 7-tier strips



$$K\{H(3,5,n)\} = \frac{1}{20160}(n+1)(n+2)^3(n+3)(25n^4 + 242n^3 + 863n^2 + 1390n + 840)$$

$$K\{H(2,6,n)\} = \frac{1}{20160}(n+1)(n+2)^2(n+3)(n+4)(31n^3 + 236n^2 + 545n + 420)$$

$$K\{M_n(L^3A^2L^2)\} = \frac{1}{5040}(n+1)(n+2)(n+3)(n+4)(34n^3 + 199n^2 + 355n + 210)$$

9.2. *The n-tuple chain* $M_n(L^3A^2L^2)$

The problem of K numbers for $M_n(L^3A^2L^2)$ was solved in a somewhat different way from the other multiple chains of the present work (Sections 7.3 and 8.2). Figure 8 shows the scheme for a suitable application of the fragmentation method. It resembles the one of Fig. 4, but differs significantly in the types of auxiliary benzenoid classes. In the present case it is obtained

$$K\{M_n(L^3A^2L^2)\} = \sum_{i=0}^{n} K\{L(n,2,i)\}\cdot K\{L(3,i)\} \tag{25}$$

where $L(3,i)$ is the well-known 3-tier parallelogram, while $L(n,2,i)$ is the 2-tier parallelogram augmented with one row. This class has been treated elsewhere [4], and it was found

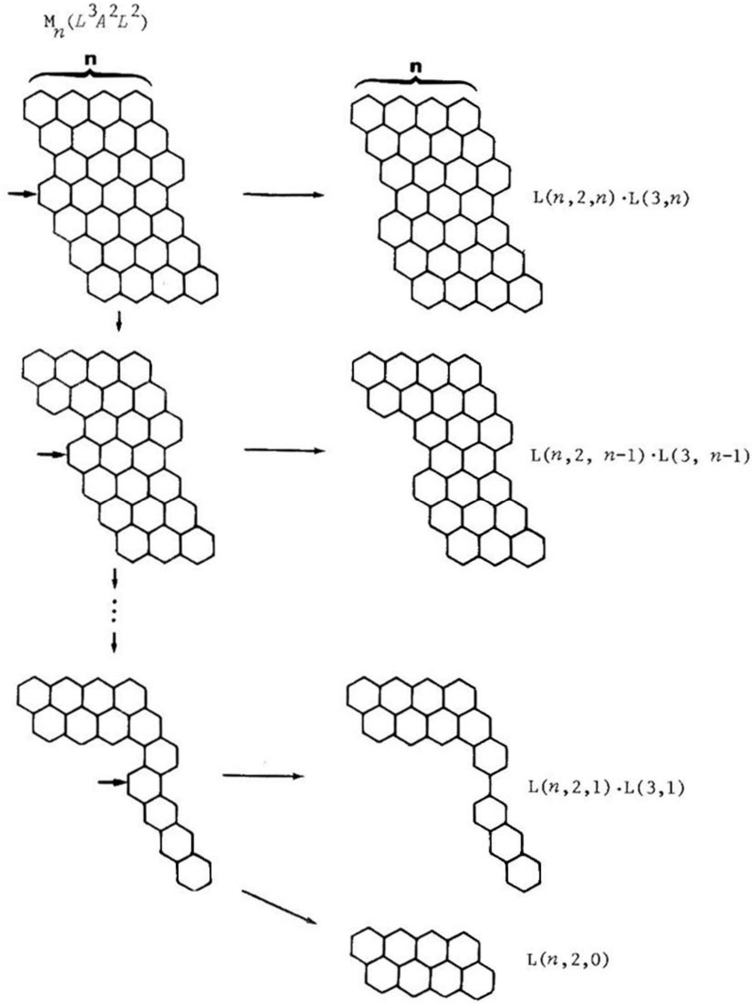


Fig. 8. The method of fragmentation applied to $M_n(L^3A^2L^2)$.

$$K\{L(n,2,l)\} = \binom{n+3}{3} - \binom{n+2-l}{3} \tag{26}$$

With the aid of this equation the right-hand side of (25) was rewritten into

$$K\{M_n(L^3A^2L^2)\} = \frac{1}{18}(3n^2 + 12n + 11)\sum_{i=0}^{n}(i+1)^2 + \frac{1}{12}(3n^2 + 10n + 7)\sum_{i=0}^{n}(i+1)^3$$
$$+ \frac{1}{36}(3n^2 + 3n - 5)\sum_{i=0}^{n}(i+1)^4 - \frac{1}{12}(n+1)\sum_{i=0}^{n}(i+1)^5 + \frac{1}{36}\sum_{i=0}^{n}(i+1)^6 \tag{27}$$

The summations were worked out to yield the net result quoted in CHART V.

9.3. *The class* $H(2,6,n)$

The method to find K for the $H(2,6,n)$ class (cf. CHART V) was the same as used for $H(2,5,n)$ of Section 8.3 (see also Sections 7.3 and 7.4). The partitioning leads to the following recurrence formula.

$$K\{H(2,6,n)\} - K\{H(2,6,\ n-1)\}$$
$$= K\{M_n(L^3A^2L^2)\} + K\{H(2,5,\ n-1)\} + K\{Di(2,4,\ n-1)\}; \quad n \geq 1 \tag{28}$$

All the required K formulas on the right-hand side are given above (see CHARTS III-V). After inserting the appropriate expressions it was arrived at

$$K\{H(2,6,n)\} - K\{H(2,6,\ n-1)\}$$
$$= \frac{1}{840}\binom{n+3}{3}(2n + 3)(31n^3 + 191n^2 + 380n + 280); \quad n \geq 1 \tag{29}$$

In the next step it was found:

$$K\{H(2,6,n)\} = \frac{1}{5040}\sum_{i=0}^{n}[62(i+1)^7 + 413(i+1)^6 + 1085(i+1)^5$$
$$+ 1505(i+1)^4 + 1253(i+1)^3 + 602(i+1)^2 + 120(i+1)] \tag{30}$$

which was reduced to the expression shown in CHART V.

9.4. *The class* $H(3,5,n)$

The approrpiate formulas from CHARTS IV and V were inserted into eqn. (24), and the expression of CHART V for $K\{H(3,5,n)\}$ emerged.

10. SEVEN-TIER OBLATE RECTANGLE: FINAL FORMULA

As the final step we insert the expressions from CHART IV and CHART V for $K\{H(3,4,n)\}$ and $K\{H(3,5,n)\}$, respectively, into eqn. (8). The resulting expression was reduced to a polynomial form; this step completes the algebraic computation of the K number for $\mathrm{Rj}(4,n)$. The final result is displayed in CHART II.

11. FULLY COMPUTERIZED METHOD

11.1. *Introduction*

Here we will outline an approach which leads to algebraic formulas for K numbers of $\mathrm{Rj}(m,n)$ with fixed m, and is entirely based on numerical analysis. The principles are generally applicable to classes of benzenoids where K is a polynomial in n. The method is convenient for computer programming. However, the below examples, although including $\mathrm{Rj}(4,n)$, are simple enough to be solved without such facilities.

It should be emphasized that the computerized method does not make the algebraic approach superfluous. The latter approach, which is treated in the preceding sections, indicates methods of wide application, it gives intermediate solutions which may be regarded as separate achievements, and it shows inter-relations between different classes of benzenoids.

The first important point is to be able to predict theoretically the degree of the polynomial

$$P_m(n) = K\{\mathrm{Rj}(m,n)\} \tag{31}$$

One has $P_1(n) = n+1$ as a trivial case, while the polynomials for $n = 2$, 3 and 4 are found in CHART II. We observe that the degrees (say d_m) of $P_m(n)$ are 1, 4, 7 and 10 for $m = 1$, 2, 3 and 4, respectively. It is reasonable to guess

$$d_m = 3m - 2 \tag{32}$$

in the general case ($m \geq 1$); the degree increases by 3 units for every unit of m. Equation (32) only as a working hypothesis is not enough for our purpose. However, it is not difficult to prove rigorously eqn. (32) by means of eqns. (1) and (5). It was done by choosing q=1 and conducting a thorough book-keeping of the highest powers of n and i. Strictly speaking we have proved $d_m \leq 3m - 2$, which is sufficient for our purpose, and where the sign of equality is highly probable.

11.2. *Polynomial in powers of n*

The approach is based on assuming a polynomial with indetermined coefficients. Thus we have in an obvious way for Rj$(2,n)$:

$$P_2(n) = a + bn + cn^2 + dn^3 + en^4 \tag{33}$$

The knowledge of five K numbers is required in order to find the coefficients. Assume that the first ones are known, i.e. $P_2(n)$ = 1, 6, 20, 50 and 105 for n = 0, 1, 2, 3 and 4, respectively (cf. TABLE 1). In particular we have taken advantage of $P_2(0) = 1$, which is the trivial case of no rings and consistent with the general formula (CHART II). This gives us 5 linear equations for the coefficients of (33). The solution is

$$a = 1,\quad b = \frac{7}{3},\ c = \frac{23}{12},\ d = \frac{2}{3},\ e = \frac{1}{12}.$$

The resulting polynomial is equivalent to the expression in CHART II.

11.3. *Application of binomial coefficeints*

As a variant of the above approach we may take advantage of expressing the polynomial in terms of binomial coefficients. As an alternative to eqn. (33) we may write

$$P_2(n) = A + B\binom{n}{1} + C\binom{n}{2} + D\binom{n}{3} + E\binom{n}{4} \tag{34}$$

This form facilitates the elimination process during the solution of the 5 linear equations for the coefficients. The computation may be set up in the shape of the Pascal triangle in the following way.

$$\begin{array}{rcl}
1 = & A & ;\quad A = 1 \\
6 = & A + B & ;\quad B = 5 \\
20 = & A + 2B + C & ;\quad C = 9 \\
50 = & A + 3B + 3C + D & ;\quad D = 7 \\
105 = & A + 4B + 6C + 4D + E & ;\quad E = 2
\end{array}$$

The resulting formula is equivalent to the previous result (CHART II).

11.4. *Assumption of partial factorization*

The number of unknowns is reduced if we assume a partial factorization of the polynomial. From the expressions of CHART II it is tempting to guess that $(n+1)$, $(n+2)^m$ and $(n+3)$ are factors in $P_m(n)$ for $m \geq 2$. Consequently we define

$$Q_m(n) = K\{\mathrm{Rj}(m,n)\}/[(n+1)(n+2)^m(n+3)]; \qquad m \geq 2 \tag{35}$$

where Q_m is a polynomial of degree $2m-4$, and

$$P_m(n) = (n+1)(n+2)^m(n+3)Q_m(n); \qquad m \geq 2 \tag{36}$$

In this work $Q_4(n)$ was determined by means of 5 unknowns using the binomial-coefficient version of the theory. Five numerical solutions had to be assumed (cf. TABLE 1); $Q_4(0) = 1/48$, $Q_4(1) = 54/648 = 1/12$, $Q_4(2) = 928/3840 = 29/120$, $Q_4(3) = 8500/15000 = 17/30$, $Q_4(4) = 52137/45360$. The following result was obtained.

$$\begin{aligned} P_4(n) &= K\{\mathrm{Rj}(4,n)\} \\ &= \frac{(n+1)(n+2)^4(n+3)}{1680}\left[34\binom{n}{4} + 119\binom{n}{3} + 161\binom{n}{2} + 105n + 35\right] \end{aligned} \tag{37}$$

Equation (37) is equivalent to the corresponding formula of CHART II. However, the general validity of eqn. (37) is not ascertained in the computerized approach because of the unproved working hypothesis of eqn. (36). A verification of eqn. (37) may be conducted in either of the two following ways: (a) to prove the hypothesis (36) for $n=4$, or (b) test eqn. (37) numerically for additional 6 values of n. A middle-way is also possible. Equation (7) shows immediately that at least $(n+2)$ is a factor in $P_4(n)$. Hence it is sufficient to test additional 5 values of n. Equation (37) gives actually the appropriate numerical values of TABLE 1 for $n = 5, 6, 7, 8$. Finally for $n=9$ the result of $P_4(9) = 22020064$ was verified to coincide with the K number for $\mathrm{Rj}(4,9)$. This completes the derivation of $K\{\mathrm{Rj}(4,n)\}$ according to the fully computerized method.

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