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ENUMERATION OF KEKULÉ STRUCTURES: PENTAGON-SHAPED BENZENOIDS - PART IV: SEVEN-TIER PENTAGONS AND RELATED CLASSES

B. N. CYVIN and S. J. CYVIN

Division of Physical Chemistry, The University of Trondheim, N-7034 Trondheim-NTH, Norway

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Abstract - A systematic terminology for classes of regular t-tier strips is given. It implies the designations: hexagon, goblet, chevron, pentagon, streamer and tower. There are six classes of mirror-symmetrical seven-tier pentagons. For three of them, which have not been treated before, the combinatorial formulas of Kekulé structure counts are derived. CHART I (pentagons) and CHART II (pentagons without apex) summarize the main results. Different methods are demonstrated for the derivation of K formulas, where K is the Kekulé structure count. The method of fragmentation is employed in different versions, and also a new method based on the John-Sachs theorem.

INTRODUCTION WITH DEFINITIONS

The studies of classes of pentagon-shaped benzenoids (or simply pentagons) have revealed many challenging problems. In the previous parts of this article series[1-3] we considered some classes of mirror-symmetrical oblate pentagons,[1] mirror-symmetrical prolate pentagons[2] and triangles.[3]

A pentagon belongs to the regular t-tier strips.[4] Assume a member of this class to be oriented in the conventional way, where the t rows are arranged from the bottom to the top. Two rims are distinguished as consisting of the first and last hexagon of each row; they are the left and right rim, respectively.

Here we are especially interested in t-tier strips where one (or both) of the rims consist of a two-segment chain. Such a two-segment chain is characterized by an LA-sequence[5] equal to L^pAL^q, where $p+q = t-1$. We will define a protruding rim and an intruding rim. If the angularly annelated

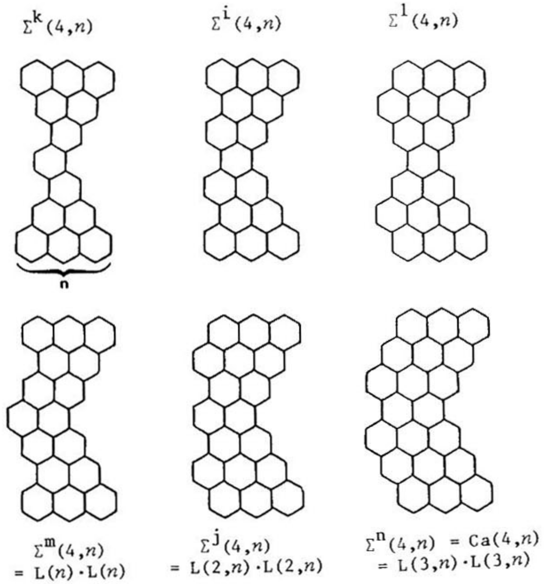
(A-mode) hexagon of a left rim is the extreme left hexagon, or if it is the extreme right hexagon in a right rim, the rim is protruding. Otherwise the rim is intruding. This terminology is convenient for a precise definition of the main classes of regular t-tier strips:

A *hexagon* has two protruding (two-segment) rims. A *goblet* has two intruding rims. A *chevron* has one protruding and one intruding rim. A *pentagon* has one protruding rim and a *streamer* one intruding.

A regular t-tier strip with no two-segment rims is a *tower*. Rectangles and multiple chains in general or zigzag chains in particular are typical examples of this wide class of benzenoids.

In the present work we have concentrated upon mirror-symmetrical seven-tier strips. There are six classes of streamers and six corresponding classes of pentagons of this kind.

The enumeration of Kekulé structures of the streamers is quickly done with. They are either essentially disconnected[4] or non-Kekuléan. In the below figure the cases of n=3 are depicted.



The general formulas for the Kekulé structure count (K for arbitrary n) read:

$$K\{\Sigma^{i}(4,n)\} = 0 \tag{1}$$

$$K\{\Sigma^{j}(4,n)\} = \frac{1}{4}\,(n+1)^{2}(n+2)^{2} \tag{2}$$

$$K\{\Sigma^{k}(4,n)\} = 0 \tag{3}$$

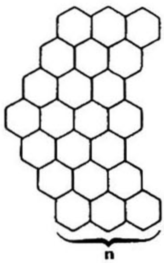
$$K\{\Sigma^{l}(4,n)\} = 0 \tag{4}$$

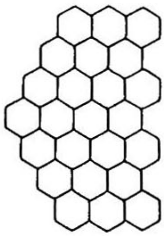
$$K\{\Sigma^{m}(4,n)\} = (n+1)^{2} \tag{5}$$

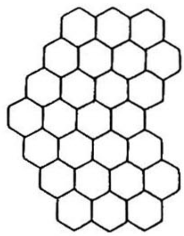
$$K\{\Sigma^{n}(4,n)\} = \frac{1}{36}(n+1)^{2}(n+2)^{2}(n+3)^{2} \tag{6}$$

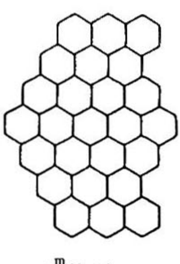
The problem of Kekulé structure counts for the corresponding pentagons (depicted below) is far more difficult.

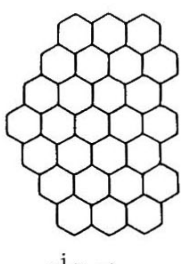
$D^{k}(4,n)$ $D^{i}(4,n)$ $D^{l}(4,n)$

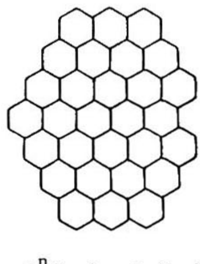










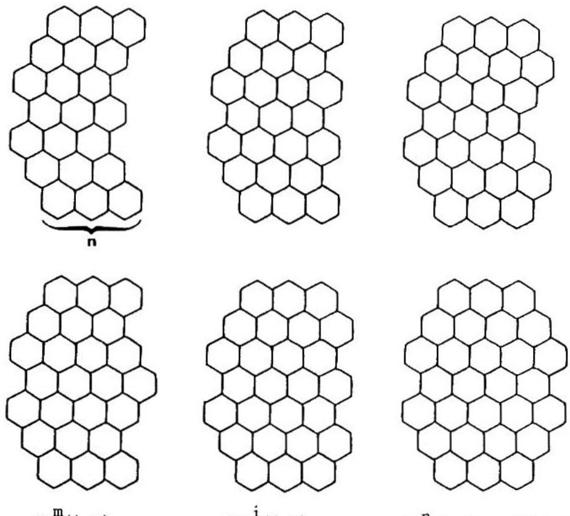


$D^{m}(4,n)$ $D^{j}(4,n)$ $D^{n}(4,n) = \mathrm{Oa}(4,n)$

The prolate pentagons, D^i, were treated in[2] Part II and the oblate, D^j, in[1] Part I. $D^n(4,n)$ is identical with the hexagon without corner,[8] Oa$(4,n)$. In the present work we report the combinatorial K formulas for $D^k(4,n)$, $D^l(4,n)$ and $D^m(4,n)$.

The derived combinatorial K formulas for five seven-tier mirror-symmetrical pentagons are collected in CHART I. In CHART II the K formulas for the corresponding pentagons without apex (see the below figures) are given.

$Da^k(4,n) = M_n(L^2A^3L^2)$ $Da^i(4,n)$ $Da^l(4,n)$



$Da^m(4,n)$ $Da^j(4,n)$ $Da^n(4,n) = Ob(4,n)$

SOME AUXILIARY BENZENOID CLASSES

Auxiliary benzenoid classes have proved to be very useful in enumerations of Kekulé structures when it is aimed at producing combinatorial formulas for benzenoid classes.

It may happen that the Kekulé structure counts (K) of two classes of regular t-tier strips, say $A(n)$ and $B(n)$, are interconnected through a sum-

CHART I - Formulas for the number of Kekulé structures (K) for classes of seven-tier pentagons

$$^{a}K\{D^{i}(4,n)\} = \frac{1}{75600}(n+1)(n+2)^{2}(n+3)^{2}(n+4)(2n+3)(2n+5)^{2}(2n+7)$$

$$^{b}K\{D^{j}(4,n)\} = \frac{1}{3628800}(n+1)(n+2)^{2}(n+3)^{3}(n+4)^{2}(n+5)(5n^{4}+60n^{3}+271n^{2}+546n+420)$$

$$^{c}K\{D^{k}(4,n)\} = \frac{1}{20160}(n+1)(n+2)^{2}(n+3)(n+4)(45n^{3}+320n^{2}+671n+420)$$

$$^{c}K\{D^{l}(4,n)\} = \frac{1}{907200}(n+1)(n+2)^{2}(n+3)^{2}(n+4)^{2}(n+5)(5n^{4}+60n^{3}+259n^{2}+474n+315)$$

$$^{c}K\{D^{m}(4,n)\} = \frac{1}{604800}(n+1)(n+2)^{2}(n+3)^{3}(n+4)^{2}(n+5)(2n+5)(9n+14)$$

[a]Ref. 2. [b]Ref. 1. [c]Present work.

CHART II - Formulas for the number of Kekulé structures (K) for classes of seven-tier pentagons without apex

$$^{a}K\{Da^{i}(4,n)\} = \frac{1}{7560}(n+1)(n+2)^{3}(n+3)(2n+3)(2n+5)(4n^{2}+16n+21)$$

$$^{b}K\{Da^{j}(4,n)\} = \frac{1}{3628800}(n+1)(n+2)^{2}(n+3)^{2}(n+4)(65n^{6}+975n^{5}+6311n^{4}+22485n^{3}+46364n^{2}+52320n+25200)$$

$$^{c}K\{Da^{k}(4,n)\} = \frac{1}{2520}(n+1)(n+2)(n+3)(45n^{4}+325n^{3}+852n^{2}+983n+420)$$

$$^{c}K\{Da^{l}(4,n)\} = \frac{1}{30240}(n+1)(n+2)^{3}(n+3)^{3}(n+4)(2n+5)(n^{2}+5n+7)$$

$$^{c}K\{Da^{m}(4,n)\} = \frac{1}{302400}(n+1)(n+2)^{2}(n+3)^{2}(n+4)(99n^{4}+815n^{3}+2616n^{2}+3820n+2100)$$

[a]Ref. 2. A misprint is corrected: the power of $(n+2)$.
[b]Present result, computed from $K\{D^{j}(4,n)\}$ of Ref. 1.
[c]Present result.

mation formula as

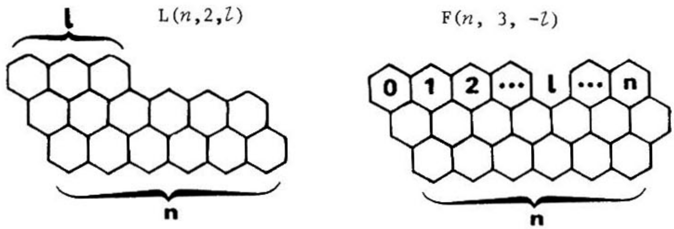
$$K\{B(n)\} = \sum_{i=0}^{n} K\{A(i)\} \tag{7}$$

Relations of this kind were already reported in the classical paper of Gordon and Davison.[6] More examples are found in the systematic treatment of five-tier strips by Cyvin et al.[4] In eqn. (7) the $A(i)$ benzenoids may be interpreted as constituting an auxiliary benzenoid class when the Kekulé structures of $B(n)$, the main class, are to be enumerated. On the other hand, if a combinatorial K formula for $B(n)$ is known, then

$$K\{A(n)\} = K\{B(n)\} - K\{B(n-1)\} \tag{8}$$

More advanced definitions of auxiliary benzenoid classes and their applications are found elsewhere.[9-18]

In the present work we will make use of two special classes of auxiliary benzenoids denoted $L(n,2,l)$ and $F(n, 3, -l)$:



The former class (L) has been studied before.[16] One has

$$K\{L(n,2,l)\} = \binom{n+3}{3} - \binom{n-l+2}{3} \tag{9}$$

The following K formula for the latter class (F) is new.

$$K\{F(n, 3, -l)\} = \frac{1}{3}(l+1)\binom{n+2}{2}\binom{n+3}{2} - 2\binom{n+3}{3}\binom{l+1}{2} + \binom{n+3}{2}\binom{l+1}{3} \tag{10}$$

THE CLASSES $D^1(4,n)$ AND $Da^1(4,n)$

The title classes are defined in the introduction. $Da^1(4,n)$ is obtained from $D^1(4,n)$ on removing the apex, i.e. the (protruding) angularly annelated hexagon of the left rim. CHART I and CHART II include the final results derived for the K numbers of benzenoids of these two classes.

The K numbers of the two classes in question are inter-related by a summation formula of the type (7), viz.

$$K\{D^1(4,n)\} = \sum_{i=0}^{n} K\{Da^1(4,i)\} \tag{11}$$

As a first task the K formula for $Da^1(4,n)$ was derived. This analysis was based on the fundamental relation

$$K\{Da^1(4,n)\} = \sum_{i=0}^{n} [K\{F(n,\ 3,\ -i)\}]^2 \tag{12}$$

It was obtained by the known enumeration techniques,[13,18] where the method of fragmentation due to Randić[19] is applied repeatedly, and the fragments are essentially disconnected benzenoids. On inserting from (10) into (12) it is obtained

$$\begin{aligned} K\{Da^1(4,n)\} = {} & \frac{1}{9}\binom{n+2}{2}^2\binom{n+3}{2}^2\sum_{i=0}^{n}(i+1)^2 - \frac{4}{3}\binom{n+2}{2}\binom{n+3}{2}\binom{n+3}{3}\sum_{i=0}^{n}(i+1)\binom{i+1}{2} \\ & + \frac{2}{3}\binom{n+2}{2}\binom{n+3}{2}^2\sum_{i=0}^{n}(i+1)\binom{i+1}{3} + 4\binom{n+3}{3}^2\sum_{i=0}^{n}\binom{i+1}{2}^2 \\ & - 4\binom{n+3}{2}\binom{n+3}{3}\sum_{i=0}^{n}\binom{i+1}{2}\binom{i+1}{3} + \binom{n+3}{2}^2\sum_{i=0}^{n}\binom{i+1}{3}^2 \end{aligned} \tag{13}$$

Here the six summations were all obtained by means of the following identities.

$$\sum_{i=0}^{n}\binom{k+i-1}{i}\binom{m+i-1}{i} = \sum_{j=1}^{k}(-1)^{k-j}\binom{n+j-1}{j-1}\binom{n+m}{m+k-j} \tag{14}$$

$$\sum_{i=1}^{n}\binom{k+i-1}{i-1}\binom{m+i-1}{i} = \sum_{j=0}^{k}(-1)^{k-j}\binom{n+j-1}{j}\binom{n+m}{m+k-j} \tag{15}$$

The identity (14) is obtained by equating two expressions for $K\{\mathrm{Ch}(k,m,n)\}$ pertaining to chevrons,[7] and (15) from $K\{\mathrm{Ch}(k+1,\ m,\ n)\} - K\{\mathrm{Ch}(k,m,n)\}$.[7] The final results for the six summations are collected in CHART III.

For the sake of brevity we show the expansion of only one of the sums of CHART III, namely the third one. We have

$$\sum_{i=0}^{n} (i+1)\binom{i+1}{3} = \binom{n+2}{4} + \sum_{i=2}^{n} i\binom{i+1}{3} \qquad (16)$$

where the last summation may be manipulated so that the identity (15) becomes applicable:

$$\sum_{i=2}^{n} i\binom{i+1}{3} = \sum_{j=1}^{n-1} (j+1)\binom{j+2}{3} = -(n+1)\binom{n+2}{3} + \sum_{j=1}^{n} \binom{3+j-1}{j-1}\binom{2+j-1}{j} \qquad (17)$$

According to (15) the last summation now becomes

$$\sum_{j=1}^{n} \binom{3+j-1}{j-1}\binom{2+j-1}{j} = -\binom{n+2}{5} + n\binom{n+2}{4} - \binom{n+1}{2}\binom{n+2}{3} + \binom{n+2}{3}\binom{n+2}{2}$$

$$= (n+1)\binom{n+3}{4} - \binom{n+3}{5} \qquad (18)$$

Inserting into (17) gives consequently

$$\sum_{i=2}^{n} i\binom{i+1}{3} = -(n+1)\binom{n+2}{3} + (n+1)\binom{n+3}{4} - \binom{n+3}{5} = (n+1)\binom{n+2}{4} - \binom{n+3}{5} \qquad (19)$$

Finally one obtains for the summation of the left-hand side of (16):

$$\sum_{i=0}^{n} (i+1)\binom{i+1}{3} = \binom{n+2}{4} + (n+1)\binom{n+2}{4} - \binom{n+3}{5} \qquad (20)$$

and consequently the pertinent expression of CHART III.

The expanded summations of CHART III were inserted into (13), and the final result rendered into the form of CHART II.

The derivation of $K\{D^1(4,n)\}$ is now a matter of routine calculations, although somewhat laborious. The expression of $K\{Da^1(4,n)\}$ according to CHART II was inserted into (11) with the result

$$K\{D^1(4,n)\} = \frac{1}{30240}\left[2\sum_{i=0}^{n}(i+1)^{11} + 33\sum_{i=0}^{n}(i+1)^{10} + 243\sum_{i=0}^{n}(i+1)^{9}\right.$$

CHART III - Some expanded summations

$$\sum_{i=0}^{n} (i+1)^2 = (n+2)\binom{n+2}{2} - \binom{n+3}{3} = \frac{1}{6}(n+1)(n+2)(2n+3)$$

$$\sum_{i=0}^{n} (i+1)\binom{i+1}{2} = \binom{n+2}{2}^2 - (n+2)\binom{n+3}{3} + \binom{n+4}{4} = \frac{1}{24}n(n+1)(n+2)(3n+5)$$

$$\sum_{i=0}^{n} (i+1)\binom{i+1}{3} = (n+2)\binom{n+2}{4} - \binom{n+3}{5} = \frac{1}{120}(n-1)n(n+1)(n+2)(4n+7)$$

$$\sum_{i=0}^{n} \binom{i+1}{2}^2 = \binom{n+2}{2}\binom{n+2}{3} - (n+2)\binom{n+3}{4} + \binom{n+4}{5}$$

$$= \frac{1}{60}n(n+1)(n+2)(3n^2+6n+1)$$

$$\sum_{i=0}^{n} \binom{i+1}{2}\binom{i+1}{3} = \binom{n+2}{3}^2 - \binom{n+2}{2}\binom{n+3}{4} + (n+2)\binom{n+4}{5} - \binom{n+5}{6}$$

$$= \frac{1}{360}(n-1)n(n+1)(n+2)(5n^2+11n+3)$$

$$\sum_{i=0}^{n} \binom{i+1}{3}^2 = \binom{n+3}{3}\binom{n+3}{4} - \binom{n+2}{2}\binom{n+4}{5} - \binom{n+2}{3}^2 + (n+2)\binom{n+4}{6} - \binom{n+5}{7}$$

$$= \frac{1}{2520}(n-1)n(n+1)(n+2)(2n+1)(5n^2+5n-9)$$

$$+ 1053\sum_{i=0}^{n}(i+1)^8 + 2976\sum_{i=0}^{n}(i+1)^7 + 5733\sum_{i=0}^{n}(i+1)^6 + 7621\sum_{i=0}^{n}(i+1)^5$$

$$+ 6897\sum_{i=0}^{n}(i+1)^4 + 4062\sum_{i=0}^{n}(i+1)^3 + 1404\sum_{i=0}^{n}(i+1)^2 + 216\sum_{i=0}^{n}(i+1)\Bigg] \quad (21)$$

The expansions of these sums are polynomials in n. All of them needed here have been reported by Chen.[14]

THE CLASSES $D^k(4,n)$ AND $Da^k(4,n)$

The combinatorial K formulas for the two title classes are found in CHART I and CHART II. The derivation of these formulas is treated very briefly in the following because the methods are basically the same as those of the preceding section.

The K numbers of the two classes are inter-related by:

$$K\{D^k(4,n)\} = \sum_{i=0}^{n} K\{Da^k(4,i)\} \tag{22}$$

The benzenoid $Da^k(4,n)$ is a multiple chain.[4] In terms of the LA-sequence it is denoted:

$$Da^k(4,n) \equiv M_n(L^2A^3L^2)$$

For this class one has the fundamental relation

$$K\{Da^k(4,n)\} = \sum_{i=0}^{n} [K\{L(n,2,i)\}]^2 \tag{23}$$

After inserting from (9) it was arrived at

$$K\{Da^k(4,n)\} = \sum_{j=0}^{n} \left[\binom{n+3}{3} - \binom{j+2}{3}\right]^2 \tag{24}$$

The summation of (24) was easily expanded after having derived the intermediate result

$$\sum_{i=0}^{n} \binom{i+2}{3}^2 = \binom{n+3}{3}\binom{n+3}{4} - \binom{n+3}{2}\binom{n+4}{5} + (n+3)\binom{n+5}{6} - \binom{n+6}{7} \tag{25}$$

It was attained at the formula

$$K\{Da^k(4,n)\} = (n+2)\binom{n+3}{3}^2 - \binom{n+3}{3}\binom{n+4}{4} - \binom{n+3}{2}\binom{n+4}{5} + (n+3)\binom{n+5}{6} - \binom{n+6}{7} \tag{26}$$

which is equivalent to the pertinent expression of CHART II. Now the derivation of $K\{D^k(4,n)\}$ is again only a matter of tedious routine. The result is entered in CHART I.

THE CLASSES $D^m(4,n)$ AND $Da^m(4,n)$

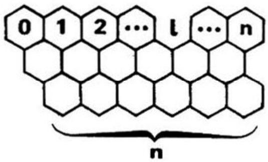
Introduction. The K numbers of the two classes $D^m(4,n)$ and $Da^m(4,n)$ are again inter-related by a summation formula of the type (5), viz.

$$K\{D^m(4,n)\} = \sum_{i=0}^{n} K\{Da^m(4,i)\} \tag{27}$$

Furthermore, the method of auxiliary classes is again applicable to $Da^m(4,n)$; its K number obeys the fundamental relation

$$K\{Da^m(4,n)\} = \sum_{i=0}^{n} [K\{B(n,\ 3,\ -i)\}]^2 \tag{28}$$

where the pertinent auxiliary benzenoid class is defined in the below figure.



$B(n,\ 3,\ -l)$

This class was also defined in a previous work,[13] but the following explicit formula for the K numbers is new.

$$K\{B(n,\ 3,\ -l)\} = (n-l+1)\binom{n+3}{3} - (n+2)\binom{n-l+2}{3} \tag{29}$$

We will not pursue this approach further in order to deduce the K formulas for the two title classes. Instead we shall demonstrate an entirely new approach, based on the John-Sachs theorem.[20] We apply it to the $D^m(4,n)$ class at once without invoking $Da^m(4,n)$. Once the K formula for $D^m(4,n)$ has been determined it is an easy task to find $K\{Da^m(4,n)\}$ as a difference in the style of eqn. (6), viz.

$$K\{Da^m(4,n)\} = K\{D^m(4,n)\} - K\{D^m(4,\ n-1)\} \tag{30}$$

Application of the John-Sachs Theorem. A new method of enumeration of Kekulé structures was recently launched.[21] It is based on the John-Sachs theorem,[20] by which the K number is identified with a determinant of a certain matrix **W**. Gutman and Cyvin[21] interpreted the matrix elements, W_{ij}, by K numbers pertaining to subgraphs of the original benzenoid. Usually they are benzenoids themselves, but may degenerate to systems with acyclic chains of edges or the empty graph. In the present application to $D^m(4,n)$ all subgraphs are either (a) parallelograms, occasionally degenerated to single linear chains of hexagons (acenes), (b) acyclic chain with K=1, or (c) the empty graph. The K formulas for the benzenoids under (a) are well known.[6]

Let the pentagon $D^m(4,n)$ be oriented so that it has four peaks and four valleys. Then it gives rise to a 4×4 determinant. CHART IV provides an illustration for n=2 as an example. The pertinent subgraphs are indicated as black silhouettes and heavy lines on the background of the original pentagon. The K numbers of the subgraphs are the **W** matrix elements W_{ij} (i,j = 1, 2, 3, 4). In the case of n=2 (CHART IV) the method yields

$$K\{D^m(4,2)\} = \begin{vmatrix} 15 & 10 & 5 & 0 \\ 6 & 10 & 10 & 0 \\ 1 & 5 & 10 & 1 \\ 0 & 1 & 5 & 3 \end{vmatrix} = 720 \qquad (31)$$

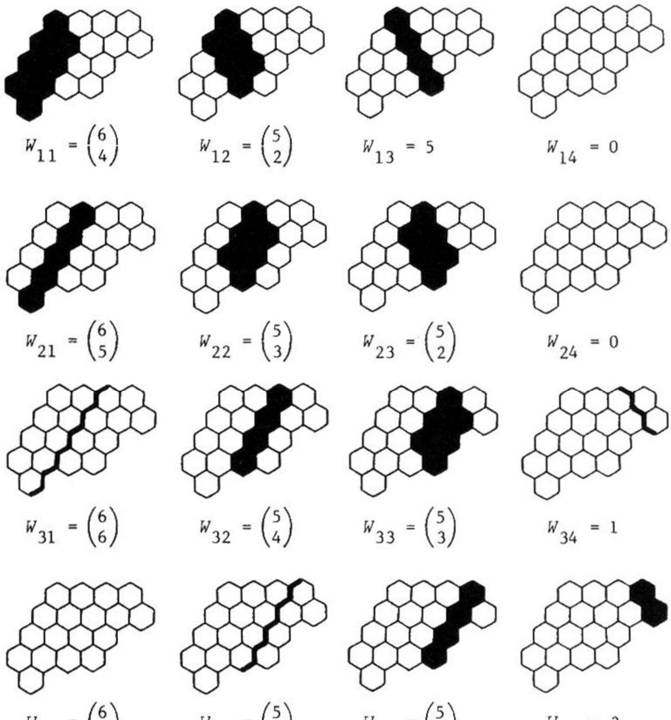
In the general case (arbitrary n):

$$K\{D^m(4,n)\} = \begin{vmatrix} \binom{n+4}{4} & \binom{n+3}{2} & (n+3) & 0 \\ \binom{n+4}{5} & \binom{n+3}{3} & \binom{n+3}{2} & 0 \\ \binom{n+4}{6} & \binom{n+3}{4} & \binom{n+3}{3} & 1 \\ \binom{n+4}{7} & \binom{n+3}{5} & \binom{n+3}{4} & (n+1) \end{vmatrix} \qquad (32)$$

The determinant (32) was expanded into:

$$K\{D^m(4,n)\} = \left[(n+1)\binom{n+3}{3} - \binom{n+3}{4}\right]\left[\binom{n+3}{3}\binom{n+4}{4} - \binom{n+3}{2}\binom{n+4}{5}\right]$$

CHART IV - Subgraphs (black) in the application of John-Sachs theorem to the pentagon $D^{m}(4,2)$. W_{ij} are K numbers



$W_{11} = \binom{6}{4}$ $W_{12} = \binom{5}{2}$ $W_{13} = 5$ $W_{14} = 0$

$W_{21} = \binom{6}{5}$ $W_{22} = \binom{5}{3}$ $W_{23} = \binom{5}{2}$ $W_{24} = 0$

$W_{31} = \binom{6}{6}$ $W_{32} = \binom{5}{4}$ $W_{33} = \binom{5}{3}$ $W_{34} = 1$

$W_{41} = \binom{6}{7}$ $W_{42} = \binom{5}{5}$ $W_{43} = \binom{5}{4}$ $W_{44} = 3$

$$- \left[(n+1)\binom{n+3}{4} - \binom{n+3}{5}\right]\left[\binom{n+3}{2}\binom{n+4}{4} - (n+3)\binom{n+4}{5}\right]$$

$$+ \left[(n+1)\binom{n+4}{6} - \binom{n+4}{7}\right]\left[\binom{n+3}{2}^2 - (n+3)\binom{n+3}{3}\right] \qquad (33)$$

No attempts were made to simplify this expression further, but all the binomial coefficients are retained in their original form as they appear in the determinant (32). However, (33) was transferred to the polynomial form with the result given in CHART I.

In conclusion it is stated that the approach invoking John-Sachs theorem turned out to be less laborious than the application of auxiliary benzenoid classes and subsequent summation. It is a convincing demonstration of the virtue of the new enumeration method,[21] of which the possible applications certainly are far from exhausted.

Final Example: Repeated Application of the Method of Fragmentation. The method of fragmentation[19] should not be discarded in spite of the conclusion of the preceding paragraph. It is a very useful method and leads often to interesting connections between K numbers of different benzenoids or benzenoid classes. Here we show an example in connection with the considered pentagon $D^{m}(4,n)$. The scheme of fragmentation which is illustrated in CHART V yields the result:

$$K\{D^{m}(4,n)\} = K\{D^{i}(4,n)\} + K\{D^{m}(4,\ n-1)\} + 2K\{D_2(3,\ 4,\ n-1)\} + K\{O(3,\ 3,\ n-1)\} \qquad (34)$$

On combining with eqn. (30) it is obtained

$$K\{Da^{m}(4,n)\} = K\{D^{i}(4,n)\} + 2K\{D_2(3,\ 4,\ n-1)\} + K\{O(3,\ 3,\ n-1)\} \qquad (35)$$

On the right-hand side of (35) the K formula for $D^{i}(4,n)$, the seven-tier prolate pentagon is known;[2] see CHART I. In the next term of (35) D_2 symbolizes a six-tier pentagon. Combinatorial K formulas for regular six-tier strips have been derived from time to time,[13,22] but not exactly for the class D_2. We give it here as an original result:

$$K\{D_2(3,\ 4,\ n-1)\} = \frac{1}{17280}\, n(n+1)^3(n+2)^3(n+3)^2(n+4) \qquad (36)$$

Finally we have the K number for the class of dihedral five-tier hexagons as the last term in (35). The appropriate formula reads[4]

$$K\{O(3,\ 3,\ n-1)\} = \frac{1}{8640}\, n(n+1)^2(n+2)^3(n+3)^2(n+4) \qquad (37)$$

In consequence, the formula for $K\{Da^{m}(4,n)\}$ is easily obtained from eqn.

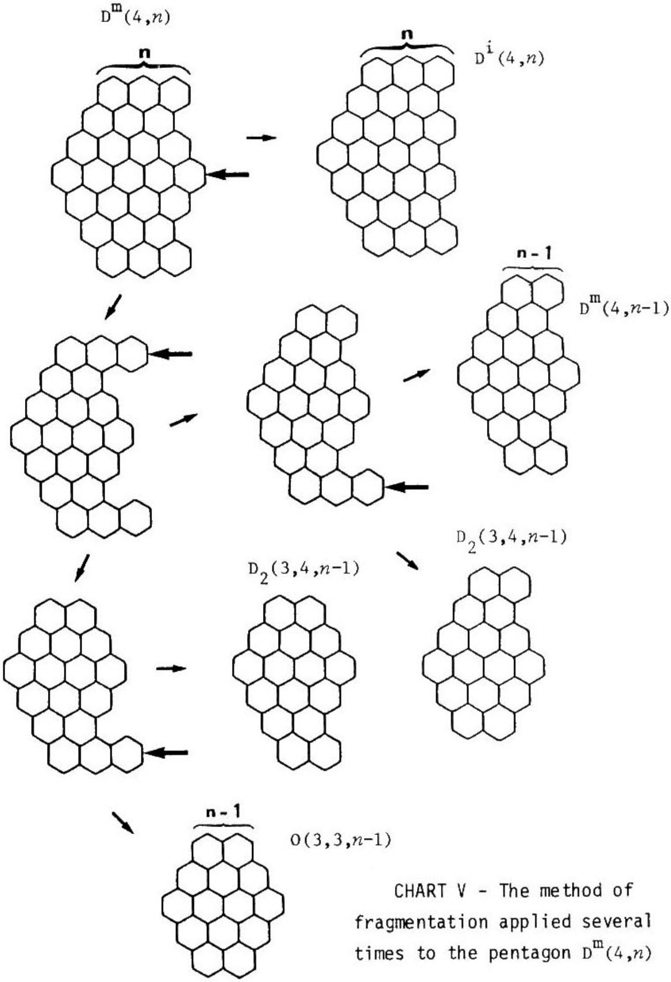


CHART V - The method of fragmentation applied several times to the pentagon $D^m(4,n)$

(35) on inserting the expressions from (36), (37) and the the first formula of CHART I. The result coincides with the last formula of CHART II.

NUMERICAL VALUES

Table 1 shows the numerical K values for the three classes of pentagons and three classes of pentagons without apices treated in the present work. Values for n up to 10 are listed.

Table 1. Numerical values of K numbers for the six specified benzenoid classes.

n	$Da^k(4,n)$	$D^k(4,n)$	$Da^l(4,n)$	$D^l(4,n)$	$Da^m(4,n)$	$D^m(4,n)$
1	25	26	52	53	45	46
2	217	243	900	953	674	720
3	1117	1360	8525	9478	5594	6314
4	4192	5552	54782	64260	31906	38220
5	12718	18270	268128	332388	140196	178416
6	33102	51372	1072224	1404612	508248	686664
7	76734	128106	3667950	5072562	1589346	2276010
8	162459	290565	11080575	16153137	4420251	6696261
9	319759	610324	30245644	46398781	11176165	17872426
10	592735	1203059	75884380	122283161	26111514	43983940

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