Number of Kekulé Structures of Five-Tier Strips

S. J. Cyvin and B. N. Cyvin
Division of Physical Chemistry, The University of Trondheim, Norway

I. Gutman
Faculty of Science, University of Kragujevac, Yugoslavia *

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Benzenoid systems called regular t-tier strips are examined. 27 classes of benzenoids belonging to the regular 5-tier strips can be distinguished. Combinatorial formulas are developed for the number of Kekulé structures of all these classes.

Introduction

The enumeration of Kekulé structures in aromatic (benzenoid) hydrocarbons has found numerous chemical applications, which have been reviewed several times [1–4]. The research in this field has been intensivated during the recent years. A part of these studies is concentrated upon peri-condensed (reticulate) benzenoids referred to as t-tier strips. In the ideal case explicit combinatorial formulas are developed for the number of Kekulé structures of different classes of these benzenoids. Three-tier strips are relatively simple and well known [5, 6]. A systematic study of four-tier strips, on the other hand, has been performed only very recently [7]. Somewhat more has previously been done for the most symmetrical five-tier strips [5, 6, 8], but far from a complete study. In the present work we wish to fill this gap. Firstly, however, we give, as a contribution to a systematic treatment, a precise definition of a regular t-tier strip. Next we present a derivation of explicit combinatorial formulas for all classes of benzenoids belonging to the regular five-tier strips. The paper illustrates several methods in the enumeration of Kekulé structures.

Definition

A regular t-tier strip is a benzenoid defined by the following two conditions.

* P.O. Box 60, Yu-34 000 Kragujevac.
Reprint requests to S. J. Cyvin, Division of Physical Chemistry, The University of Trondheim, N-7034 Trondheim-NTH, Norway.

(a) It consists of t tier fused chains (rows), conventionally drawn horizontally, where the bottom and top chain should have the same length in terms of the number of hexagons, say n.

(b) The (vertical) rims should each consist of a connected chain of t hexagons, of which any *LA*-sequence [9, 10] is permitted.

This definition sorts out a limited number of classes for every t value, and yet it embraces the conventional classes as parallelograms, hexagons, chevrons, etc. [5–8].

As a first illustration of this definition we give examples of (non-regular) five-tier strips, which do not obey the above conditions. Either (a) or (b) or both of them may be violated; cf. Figure 1.

Regular Five-Tier Strips

The regular five-tier strips consist of twenty-seven classes, which may be divided into three series (I–III) and derived from the classes of hexagons, say $O(k, m, n)$; cf. Figure 2. If $k = m$ the hexagon is referred to as dihedral; if all parameters (k, m, n) are different as centro-symmetrical.

Ohkami and Hosoya [8] were probably the first to suggest a study of the latter type. If $k = 1$ the hexagon degenerates into the $m \times n$ or $L(m, n)$ parallelogram. For a t-tier strip

$$k + m = t + 1 . \tag{1}$$

(I) $k = m = 3$. The leading class of hexagons is given by $O(3, 3, n)$; a member of any other class of this series is a sub-benzenoid of $O(3, 3, n)$. The top and bottom rows are unshifted.

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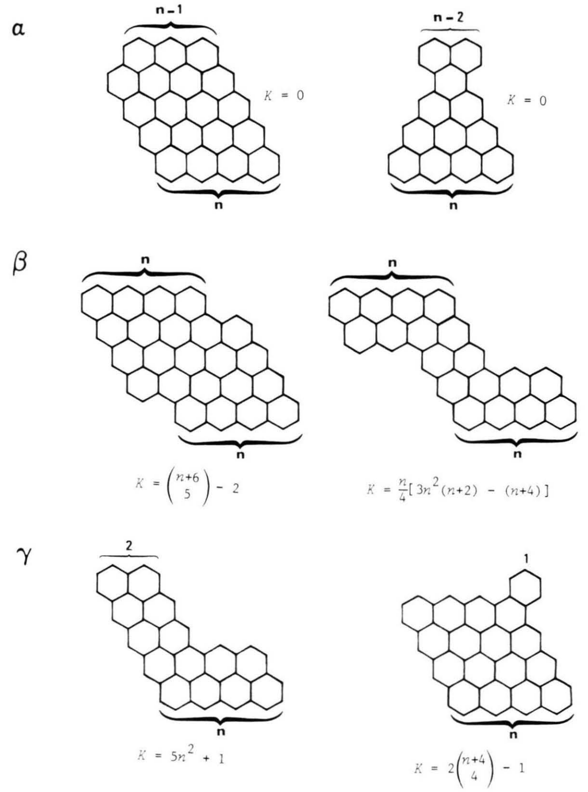

Fig. 1. Classes of non-regular 5-tier strips: (α) The condition (a) is violated. Both of the benzenoids are non-Kekuléan. The one to left has an odd number of vertices; the one on the right-hand side has an even number of vertices, but not the same number of black and white ones; cf. the section about non-Kekuléan structures. (β) The condition (b) is violated. (γ) Both conditions (a) and (b) are violated.

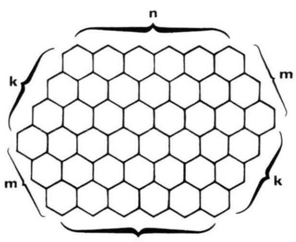

Fig. 2. The definition of a hexagon-shaped benzenoid in terms of three parameters (k, m, n).

(II) $k = 2$, $m = 4$. The leading hexagon is $O(2, 4, n)$. The top and bottom rows are shifted by one hexagon.

(III) $k = 1$, $m = 5$. This series consists of the only class $O(1, 5, n) = L(5, n)$. The top-bottom shift is of the length of two hexagons.

Figures 3 and 4 show the ten plus six classes within the series **(I)**. Figure 5 shows the ten classes within the series **(II)**; they are analogous to the classes of Figure 3. Finally the parallelogram of the series **(III)** is depicted in Figure 6.

General Formulas: Hexagons and Chevrons

Within the regular t-tier strips the hexagon-shaped and chevron-shaped benzenoids are the only three-parameter classes for which the number of Kekulé structures (K) is known in terms of general explicit formulas.

When $K\{B\}$ denotes the K number of the benzenoid B, one has

$$K\{O(k, m, n)\} = \prod_{i=0}^{k-1} \binom{m+n+i}{n} \bigg/ \binom{n+i}{n}. \quad (2)$$

This formula for the hexagon in the general case was first given by Cyvin [7] as a generalization of a formula pertaining to dihedral hexagons [5]. The three parameters (k, m, n) in (2) are completely permutable.

For the chevron [5, 7] a general formula reads

$$K\{Ch(k, m, n)\} = \sum_{i=0}^{n} \binom{k+i-1}{i} \binom{m+i-1}{i}. \quad (3)$$

Here k and m are interchangeable, but n is unique. Therefore an alternative formula is very useful, where the summation to n is replaced by a summation to k. It is presented here for the first time:

$$K\{Ch(k, m, n)\} \quad (4)$$
$$= \sum_{j=\max(1, k-n)}^{k} (-1)^{k-j} \binom{n+j-1}{n} \binom{n+m}{n-k+j}.$$

An application of (2) gives readily

$$\textbf{(I-1)} \quad K\{O(3, 3, n)\} = \frac{1}{40} \binom{n+3}{3} \binom{n+4}{3} \binom{n+5}{3}$$
$$= \frac{1}{8640} (n+1)(n+2)^2(n+3)^3(n+4)^2(n+5). \quad (5)$$

The polynomial form in (5) was also derived by Ohkami and Hosoya [8]. Similarly we obtain

$$\textbf{(II-1)} \quad K\{O(2, 4, n)\} = \frac{1}{5} \binom{n+4}{4} \binom{n+5}{4} \quad (6)$$
$$= \frac{1}{2880} (n+1)(n+2)^2(n+3)^2(n+4)^2(n+5).$$

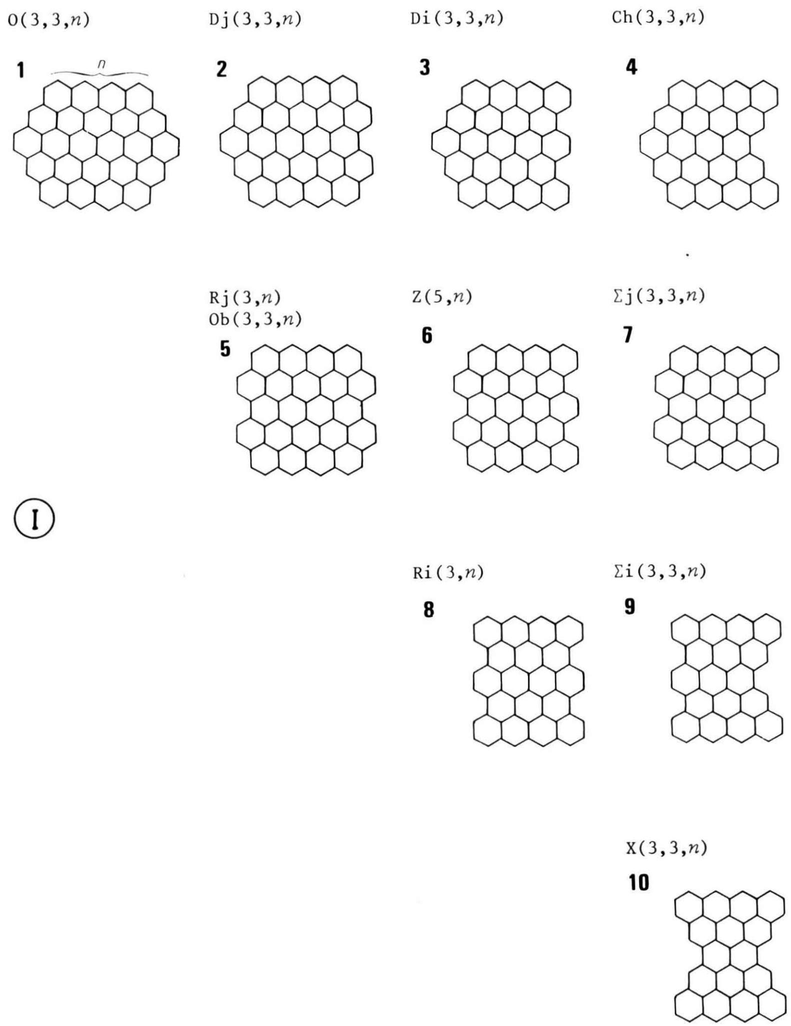

Fig. 3. Ten classes of regular 5-tier strips belonging to the series **(I)**. The drawings have $n = 4$.

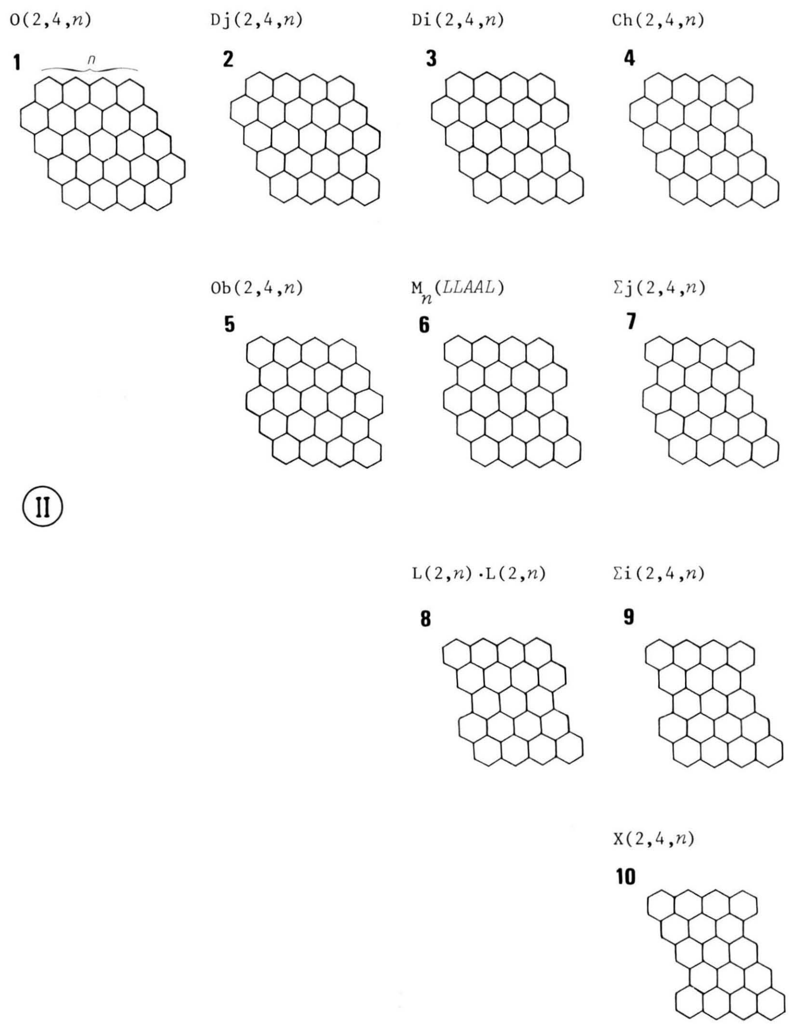

Fig. 5. The existing ten classes of regular 5-tier strips belonging to the series **(II)**. The drawings have $n = 4$.

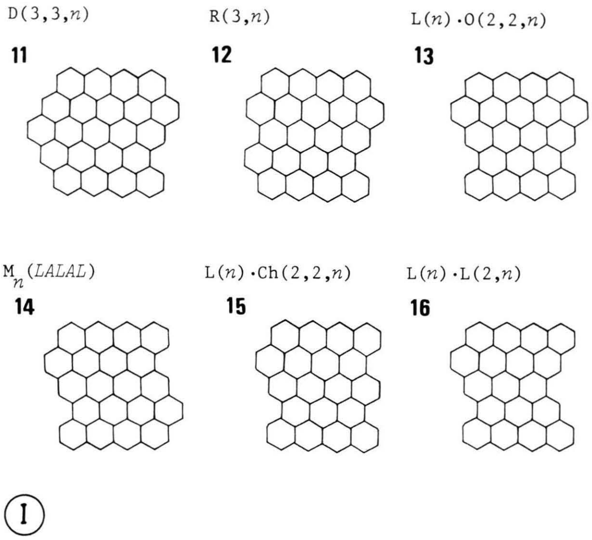

Fig. 4. Additional six classes of regular 5-tier strips belonging to the series **(I)**. The drawings have $n = 4$.

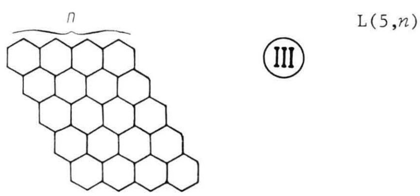

Fig. 6. The parallelogram $5 \times n$, where $n = 4$. It constitutes the series **(III)** of regular 5-tier strips.

Boldface figures in parentheses, as in front of (5) and (6), refer to Figures 3–6.

The application of the general formulas to chevrons (**4**) renders an eludicating example. On application of (3) one obtains

$$\textbf{(I-4)}\quad K\{\mathrm{Ch}(3,3,n)\} = \sum_{i=0}^{n} \binom{i+2}{2}^2 = \frac{1}{4}\sum_{i=0}^{n} (i+1)^2(i+2)^2 \qquad (7)$$
$$= \frac{1}{60}(n+1)(n+2)(n+3)(3n^2+12n+10).$$

From (4), on the other hand, one obtains

$$\textbf{(I-4)}\quad K\{\mathrm{Ch}(3,3,n)\} \qquad (8)$$
$$= \binom{n+2}{2}\binom{n+3}{3} - (n+1)\binom{n+3}{4} + \binom{n+3}{5},$$

which already is an explicit formula, although in terms of binomial coefficients. It reduces indeed to the same polynomial form as in (7). For the chevron of series **(II)**, (4) is again much easier to apply than (3) and gives

$$\textbf{(II-4)}\quad K\{\mathrm{Ch}(2,4,n)\} = (n+1)\binom{n+4}{4} - \binom{n+4}{5} \qquad (9)$$
$$= \frac{1}{120}(n+1)(n+2)(n+3)(n+4)(4n+5).$$

Parallelograms and Essentially Disconnected Benzenoids

Parallelogram

For the parallelogram-shaped benzenoid, L(m,n), the number of Kekulé structures is one of the classical results [5];

$$K\{L(m,n)\} = \binom{m+n}{n}. \qquad (10)$$

Hence

$$\textbf{(III)}\quad K\{\mathrm{L}(5,n)\} = \binom{n+5}{5} \qquad (11)$$
$$= \frac{1}{120}(n+1)(n+2)(n+3)(n+4)(n+5).$$

Essentially Disconnected Parallelograms

A number of classes of the regular five-tier strips contain essentially single bonds and may be referred to as essentially disconnected. First we consider the benzenoids whose fragments are parallelograms, occasionally reduced to single chains. For the latter case

$$K\{\mathrm{L}(n)\} = K\{\mathrm{L}(1,n)\} = n+1. \qquad (12)$$

This is a special case of (10) for $m = 1$. The K numbers are obtained by (10) and (12), and multiplication of the individual K's for the fragments. In summary we obtain:

$$\textbf{(I-7)}\quad K\{\Sigma j(3,3,n)\} = \binom{n+2}{2}^2 = \tfrac{1}{4}(n+1)^2(n+2)^2, \qquad (13)$$

$$\textbf{(I-8)}\quad K\{\mathrm{Ri}(3,n)\} = (n+1)^3, \qquad (14)$$

$$\textbf{(I-9)}\quad K\{\Sigma \mathrm{i}(3,3,n)\} = (n+1)^2, \qquad (15)$$

(I-16) $K\{L(n)\cdot L(2,n)\} = (n+1)\binom{n+2}{2}$

$$= \tfrac{1}{2}(n+1)^2(n+2), \qquad (16)$$

(II-7) $K\{\Sigma\, j(2,4,n)\} = (n+1)\binom{n+3}{3}$

$$= \tfrac{1}{6}(n+1)^2(n+2)(n+3), \qquad (17)$$

(II-8) $K\{L(2,n)\cdot L(2,n)\} = \binom{n+2}{2}^2$

$$= \tfrac{1}{4}(n+1)^2(n+2)^2, \qquad (18)$$

(II-9) $K\{\Sigma\, i(2,4,n)\} = (n+1)\binom{n+2}{2}$

$$= \tfrac{1}{2}(n+1)^2(n+2), \qquad (19)$$

(II-10) $K\{X(2,4,n)\} = (n+1)^2. \qquad (20)$

Other Essentially Disconnected Benzenoids

In two instances we encounter essentially disconnected benzenoids with fragments others than parallelograms, viz. three-tier hexagon, O(2, 2, n) and chevron, Ch(2, 2, n). The K numbers for the classes of these fragments are well known [5], and also (2)–(4) are applicable. Our result is:

(I-13) $K\{L(n)\cdot O(2,2,n)\}$

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

$$= \frac{1}{12}(n+1)^2(n+2)^2(n+3), \qquad (21)$$

(I-15) $K\{L(n)\cdot Ch(2,2,n)\}$

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

$$= \tfrac{1}{6}(n+1)^2(n+2)(2n+3). \qquad (22)$$

Non-Kekuléan Structures

The principal difference between **(I-10)** and **(II-10)** should be noticed; while X(2, 4, n) is essentially disconnected and Kekuléan, X(3, 3, n) is non-Kekuléan:

(I-10) $K\{X(3,3,n)\} = 0 \qquad (23)$

for all values of n. In a benzenoid system (drawn so that some of its edges are vertical) we may distinguish "peaks" – vertices which lie above all their first neighbours – and "valleys" – vertices which lie below all their first neighbours. The equality of the number of peaks with the number of valleys is a necessary condition for the existence of Kekulé structures. The benzenoids on Fig. 1 (α) have three and two peaks, respectively, and four valleys each. This explains why $K = 0$ has been found for them. The above condition, however, is not sufficient, as shown by the example of X(3, 3, n). This benzenoid has both n peaks and n valleys. The member X(3, 3, 3) coincides with one of Gutman's [11] examples of non-Kekuléan structures. A detailed treatise on the recognition of Kekuléan and non-Kekuléan benzenoids is to be published elsewhere [12].

Multiple Chains

A multiple chain is defined as fused parallel chains, which may have kinks in alternating left-right-left-... manner. The concept of *LA*-sequences [9, 10] is applicable to multiple chains. In our context (t-tier strips) the multiple chains reveal themselves by having all rows of the equal length (n hexagons). There are six classes of multiple chains in our collection (5-tier strips): the parallelogram **(III)**, the chevrons **(I-4)** and **(II-4)**, the zig-zag chain **(I-6)**, along with **(II-6)** $M_n(LLAAL)$ and **(I-14)** $M_n(LALAL)$. In this notation, particularly designed for multiple chains, one has

(III) $L(5,n) = M_n(LLLLL)$,

(II-4) $Ch(2,4,n) = M_n(LLLAL)$,

(I-4) $Ch(3,3,n) = M_n(LLALL)$,

(I-6) $Z(5,n) = M_n(LAAAL)$.

A general theory for the K numbers of multiple chains has not been developed. Preliminary (so far unpublished) findings have resulted in the following formulas:

(I-6) $K\{Z(5,n)\} = (n+1)\left[\binom{n+2}{2}^2 - \binom{n+3}{4}\right]$

$$- \binom{n+2}{2}\binom{n+2}{3} + \binom{n+3}{5} \qquad (24)$$

$$= \frac{1}{30}(n+1)(n+2)(2n+3)(2n^2+6n+5),$$

(II-6) $K\{M_n(LLAAL)\} = \binom{n+2}{2}\binom{n+3}{3} - \binom{n+4}{5}$

$$= \frac{1}{120}(n+1)(n+2)(n+3)(9n^2+26n+20), \quad (25)$$

(I-14) $K\{M_n(LALAL)\}$

$$= (n+1)\left[(n+1)\binom{n+3}{3} - 2\binom{n+3}{4}\right] + \binom{n+3}{5}$$
$$= \frac{1}{120}(n+1)(n+2)(n+3)(11n^2+29n+20). \quad (26)$$

The polynomial form of (24) was deduced in a different way by Gutman and Cyvin [13], while (25) and (26) are new.

Summation- and Recurrence Formulas

General

Many of the considered classes of benzenoids are inter-connected with respect to their number of Kekulé structures. The underlying theory is well known in the enumeration techniques of Kekulé structures [14], and has been applied previously to t-tier strips specifically by Yen [6]. If we, for instance, focus the attention upon the utter-most right- (or left-) hand bond in **(I-1)** we arrive at

$$K\{O(3,3,n)\} = K\{O(3,3,n-1)\} + K\{Dj(3,3,n)\}. \quad (27)$$

By successive application of this recurrence formula and the initial conditions

$$K\{O(3,3,0)\} = K\{Dj(3,3,0)\} = 1$$

we obtain the summation formula

$$K\{O(3,3,n)\} = \sum_{i=0}^{n} K\{Dj(3,3,i)\}. \quad (28)$$

Altogether we have derived the following equations of the types (27) and (28):

$$K_n\{\mathbf{1}\} = \sum_{i=0}^{n} K_i\{\mathbf{2}\}, \quad (29)$$

$$K_n\{\mathbf{2}\} = K_n\{\mathbf{1}\} - K_{n-1}\{\mathbf{1}\}, \quad (30)$$

$$K_n\{\mathbf{2}\} = \sum_{i=0}^{n} K_i\{\mathbf{5}\}, \quad (31)$$

$$K_n\{\mathbf{3}\} = \sum_{i=0}^{n} K_i\{\mathbf{6}\}, \quad (32)$$

$$K_n\{\mathbf{4}\} = \sum_{i=0}^{n} K_i\{\mathbf{7}\}, \quad (33)$$

$$K_n\{\mathbf{5}\} = K_n\{\mathbf{2}\} - K_{n-1}\{\mathbf{2}\}, \quad (34)$$

$$K_n\{\mathbf{6}\} = K_n\{\mathbf{3}\} - K_{n-1}\{\mathbf{3}\}, \quad (35)$$

$$K_n\{\mathbf{7}\} = K_n\{\mathbf{4}\} - K_{n-1}\{\mathbf{4}\}. \quad (36)$$

Here the boldface figures refer to Fig. 3 or 5. The equations apply to both series **(I)** and **(II)**. Thus, for instance, when (29) is used for **(I-1)** and **(I-2)** it coincides with (28). Finally we have a connection between two of the classes from Fig. 4:

$$K_n\{\textbf{I-11}\} = \sum_{i=0}^{n} K_i\{\textbf{I-12}\}, \quad (37)$$

$$K_n\{\textbf{I-12}\} = K_n\{\textbf{I-11}\} - K_{n-1}\{\textbf{I-11}\}. \quad (38)$$

Application of Hexagons

The K formulas for the hexagons **(1)** are known; cf. (5) and (6). When they are applied in (30) we obtain first

(I-2) $K\{Dj(3,3,n)\} = \frac{1}{40}\binom{n+3}{3}\binom{n+4}{3}\binom{n+5}{3}$

$$- \frac{1}{40}\binom{n+2}{3}\binom{n+3}{3}\binom{n+4}{3}$$
$$= \frac{1}{2880}(n+1)(n+2)^2(n+3)^2(n+4) \cdot (3n^2+15n+20). \quad (39)$$

For this class Yen [6] has given a considerably more complicated equation in terms of binomial coefficients, while Ohkami and Hosoya [8] arrived at the polynomial form of (39) by a different method involving laborious algebraic computations, which were executed by a computer program. In the series **(II)** we obtain a new formula, viz.

(II-2) $K\{Dj(2,4,n)\}$

$$= \frac{1}{5}\binom{n+4}{4}\binom{n+5}{4} - \frac{1}{5}\binom{n+3}{4}\binom{n+4}{4}$$
$$= \frac{1}{720}(n+1)(n+2)^2(n+3)^2(n+4)(2n+5). \quad (40)$$

With this newly acquired knowledge of K formulas for oblate pentagons (**2**) we obtain those of the hexagons without two corners (**5**) by means of (34). The final results in polynomial form are:

$$\textbf{(I-5)}\quad K\{\mathrm{Rj}(3,n)\} = K\{\mathrm{Ob}(3,3,n)\} \tag{41}$$

$$= \frac{1}{120}(n+1)(n+2)^3(n+3)(n^2+4n+5),$$

$$\textbf{(II-5)}\quad K\{\mathrm{Ob}(2,4,n)\} \tag{42}$$

$$= \frac{1}{360}(n+1)(n+2)^2(n+3)(7n^2+28n+30).$$

Equation (41) has been given previously [5, 6, 8], while (42) is new.

Application of Chevrons

Equations (33) and (36) give the connection between the K values of chevrons and oblate streamers. These are all known according to (8), (9), (13) and (16). Hence (33) and (36) do not give new information, but they are useful for checking the results.

Application of the Zig-Zag Chain

The case of **(I-3)**, prolate pentagon, is one of the most difficult among the regular five-tier strips. The problem of K has not been solved before for this class. We have not found any easier method than the crude application of (32) together with (24):

$$\textbf{(I-3)}\quad K\{\mathrm{Di}(3,3,n)\} = \sum_{i=0}^{n} K\{\mathrm{Z}(5,i)\}$$

$$= \frac{2}{15}\sum_{i=0}^{n}(i+1)^5 + \frac{1}{3}\sum_{i=0}^{n}(i+1)^4$$

$$+ \frac{1}{3}\sum_{i=0}^{n}(i+1)^3 + \frac{1}{6}\sum_{i=0}^{n}(i+1)^2 \tag{43}$$

$$+ \frac{1}{30}\sum_{i=0}^{n}(i+1)$$

$$= \frac{1}{180}(n+1)(n+2)^2(n+3)(2n+3)(2n+5).$$

Application of a Multiple Chain

The formula for **(II-3)** may be derived in the same crude way as above: application of (32) together with the polynomial form of (25). Instead we have arrived at the result in a more interesting way, and perhaps also easier. By means of (32) and the binomial-coefficient form of (25) we obtain

$$K\{\mathrm{Di}(2,4,n)\} = \sum_{i=0}^{n} K\{\mathrm{M}_i(LLAAL)\}$$

$$= \sum_{i=0}^{n}\binom{i+2}{2}\binom{i+3}{3} - \sum_{i=0}^{n}\binom{i+4}{5}. \tag{44}$$

The first summation of the right-hand side is recognized as the K number of a chevron when written in the following way:

$$\sum_{i=0}^{n}\binom{3+i-1}{i}\binom{4+i-1}{i} = K\{\mathrm{Ch}(3,4,n)\} \tag{45}$$

$$= \binom{n+4}{6} - (n+1)\binom{n+4}{5} + \binom{n+2}{2}\binom{n+4}{4}.$$

It is referred to (3). In the last part of (45), however, we have used the chevron formula (4). The last summation in (44) is more manageable. Notice first that it may be started equally well from $i = 1$. Furthermore,

$$\sum_{i'=1}^{n}\binom{i'+4}{5} = \sum_{i=0}^{n-1}\binom{i+5}{5} = \binom{n+5}{6}$$

$$= K\{\mathrm{L}(6, n-1)\}. \tag{46}$$

Here we have arrived at an interesting result. The considered benzenoid **(II-3)** has the K number equal to the difference between the K numbers of two other benzenoids, which belong to the six-tier strips. The situation is illustrated in Figure 7. The desired formula for the prolate pentagon is now obtained, according to (44), by subtracting (46) from (45). This result is already an explicit formula, though in terms of binomial coefficients. By elementary manipulations we have arrived at

$$\textbf{(II-3)}\quad K\{\mathrm{Di}(2,4,n)\}$$

$$= \binom{n+2}{2}\binom{n+4}{4} - (n+2)\binom{n+4}{5} \tag{47}$$

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

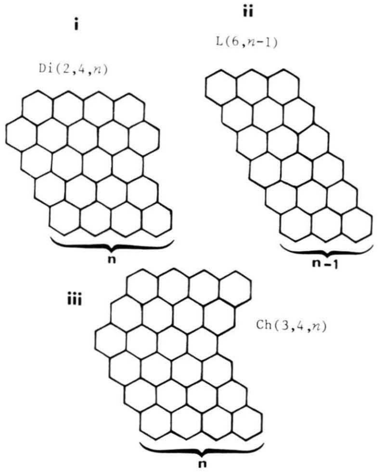

Fig. 7. The classes of benzenoids: (i) Prolate pentagons Di (2, 4, n), (ii) parallelograms L (6, $n-1$), and (iii) chevrons Ch (3, 4, n). It was found (see the text): $K\{\mathrm{i}\} + K\{\mathrm{ii}\} = K\{\mathrm{iii}\}$.

Intermediate Rectangle and Pentagons

So far we are left with two classes, the intermediate pentagon, D (3, 3, n), and intermediate rectangle, R (3, n), viz. **(I-11)** and **(I-12)**, respectively. Their numbers of Kekulé structures are interconnected according to (37) and (38). The pentagon **(I-11)** comes in a sense in-between the oblate pentagon **(I-2)** with indentation outwards, Dj (3, 3, n), and the prolate pentagon **(I-3)** with indentation inwards, Di (3, 3, n). In the same sense the intermediate rectangle **(I-12)** fits in-between the oblate rectangle **(I-5)**, Rj (3, n), and the zig-zag chain **(I-6)**, Z (5, n).

The previously applied techniques in enumeration of Kekulé structures [14] lead to the desired formula for R (3, n) when applied twice. In the first place we obtained a resolution of R (3, n) into the zig-zag chain Z (5, n) and the special benzenoid (iv) depicted in Figure 8. The figure illustrates the next step of resolution (iv) into the two benzenoids of identified classes. The net result gives

$$K\{\mathrm{R}(3,n)\} - K\{\mathrm{R}(3,n-1)\} = K\{\mathrm{Z}(5,n)\} + K\{\mathrm{D}(2,3,n-1)\}. \quad (48)$$

This recurrence formula leads to the summation

$$K\{\mathrm{R}(3,n)\} = \sum_{i=0}^{n} K\{\mathrm{Z}(5,i)\} + \sum_{i=0}^{n-1} K\{\mathrm{D}(2,3,i)\}. \quad (49)$$

The first summation on the right-hand side of (49) is identical with (32). The last summation is concerned with four-tier strips [7]. A relation analogous to (28) holds also in this case, viz.

$$K\{\mathrm{O}(2,3,n)\} = \sum_{i=0}^{n} K\{\mathrm{D}(2,3,i)\} = \frac{1}{4}\binom{n+3}{3}\binom{n+4}{3}. \quad (50)$$

Hence, with the aid of (43), (49) and (50):

(I-12) $K\{\mathrm{R}(3,n)\}$

$$= K\{\mathrm{Di}(3,3,n)\} + K\{\mathrm{O}(2,3,n-1)\} = \frac{1}{240}(n+1)(n+2)^2(n+3)(7n^2+23n+20). \quad (51)$$

We wish to mention that the same methods may lead to an alternative decomposition of R (3, n); similarly to (48) one also has

$$K\{\mathrm{R}(3,n)\} - K\{\mathrm{R}(3,n-1)\} = K\{\mathrm{M}_n(LALAL)\} + K\{\mathrm{L}(n)\cdot\mathrm{O}(2,2,n-1)\} \quad (52)$$

and consequently

$$K\{\mathrm{R}(3,n)\} = \sum_{i=0}^{n} K\{\mathrm{M}_i(LALAL)\} + \sum_{i=0}^{n-1} K\{\mathrm{L}(i+1)\}\cdot\{\mathrm{O}(2,2,i)\}. \quad (53)$$

In this case, however, the two summations on the right-hand side are not immediately accessible.

The last formula, which pertains to D (3, 3, n), was obtained in the tedious way analogous to (43).

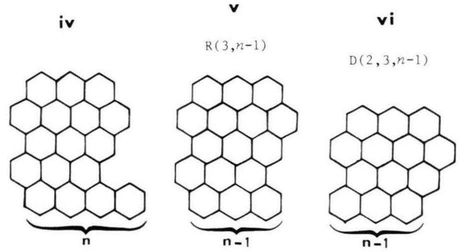

Fig. 8. Three benzenoid classes encountered during the derivation of the K number for R (3, n). It was found (see the text): $K\{\mathrm{iv}\} = K\{\mathrm{v}\} + K\{\mathrm{vi}\}$.

Equation (37) together with (51) gives

$$\textbf{(I-11)}\quad K\{D(3,3,n)\} = \sum_{i=0}^{n} K\{R(3,i)\} = \frac{1}{720}(n+1)(n+2)^2 \cdot (3n^4 + 35n^3 + 149n^2 + 273n + 180)\,. \qquad (54)$$

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