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THE NUMBER OF KEKULÉ STRUCTURES FOR RECTANGLE-SHAPED BENZENOIDS - PART V

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The number of Kekulé structures (K) for oblate (and prolate) rectangles are treated by means of the John-Sachs theorem. A general formulation for $K\{\mathrm{R}^{\mathrm{j}}(m,n)\}$ in terms of a determinant is achieved. Finally the auxiliary benzenoid classes related to $\mathrm{R}^{\mathrm{j}}(m,n)$ are considered.

INTRODUCTION

Combinatorial formulas of K, the number of Kekulé structures, for oblate rectangle-shaped benzenoids (or simply rectangles), $\mathrm{R}^{\mathrm{j}}(m,n)$, represent some of the more difficult problems in the enumeration of Kekulé structures. Formulas of $K\{\mathrm{R}^{\mathrm{j}}(m,n)\}$ with fixed values of m are long known for the lowest values of this parameter, viz. m=2 [1] and m=3 [1-4]. For higher m values laborious methods had to be devised before the problems could be solved. The K formulas for m=4 [5], m=5 [6], m=6 [7] and m=7 [8] have been reported.

In the present work we employ a newly developed K enumeration method, which is based on a theorem by John and Sachs [9]. The result is a general formulation of $K\{\mathrm{R}^{\mathrm{j}}(m,n)\}$ in terms of a determinant. The special cases of m = 4, 5, 6 and 7 give the previous results [5-8] with less labor, and there is no hindrance against an extension to still higher values of m.

GENERAL DESCRIPTION OF THE METHOD

According to John and Sachs [9] a K number of a Kekuléan benzenoid B is obtainable as the determinant of a matrix **W** whose elements W_{ij} are obtained by counting the monotonic paths starting from the i-th peak and ending at the j-th valley. Gutman and Cyvin [10] increased the practical applicability of this rule by identifying the W_{ij} elements with K numbers of certain subgraphs in B. They are either benzenoids themselves or degenerate systems consisting of or containing acyclic edges. An element may also vanish, corresponding to the empty graph. More precisely, W_{ij} is the intersection of two graphs, the so-called wetting area of the i-th peak, $R(p_i)$, and the catchment area of the j-th valley, $R(v_j)$.

APPLICATION TO PROLATE RECTANGLES

For a prolate rectangle [5], $R^i(m,n)$, which is essentially disconnected [4], the K formula is well known [2], viz. $K\{R^i(m,n)\} = (n+1)^m$.

An oblate rectangle [5], $R^j(m,n)$, may be interpreted as a prolate rectangle $R^i(m-1,\ n+1)$ augmented with two rows of n hexagons each at the top and the bottom; see Fig. 1.

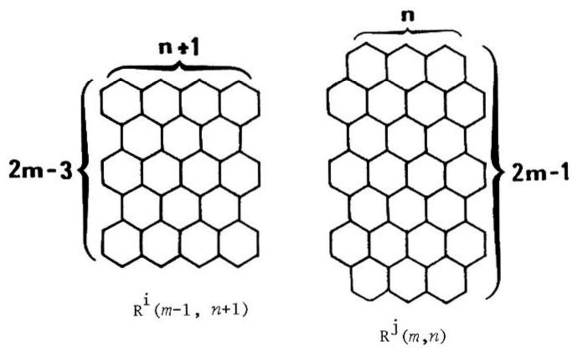

Fig. 1. The oblate rectangle, $R^j(m,n)$, generated from the prolate rectangle $R^i(m-1,\ n+1)$. Figures for m=4 and n=3 are depicted.

Therefore it is reasonable to apply the described method to the prolate rectangle first. The further development shows that it will be a part of the solution for $R^j(m,n)$.

In order to apply the present method the $R^i(m-1,\ n+1)$ rectangle should be oriented in a non-conventional way as shown in Fig. 2. In this orientation it has m-1 peaks and m-1 valleys. Without going into further details we specify the $(m-1)\times(m-1)$ determinant obtained as a result of the analysis:

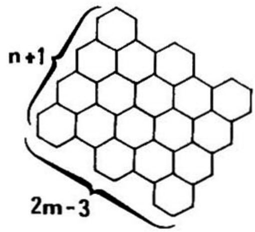

Fig. 2. Orientation of the prolate rectangle suitable for the application of the present method.

$$D^{\mathrm{i}} = \begin{vmatrix} \binom{n+2}{n+1} & \binom{n+3}{n} & \binom{n+4}{n-1} & \cdots & \binom{n+m}{n-m+3} \\ 0 & \binom{n+2}{n+1} & \binom{n+3}{n} & \cdots & \binom{n+m-1}{n-m+4} \\ 0 & 0 & \binom{n+2}{n+1} & \cdots & \binom{n+m-2}{n-m+5} \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ 0 & 0 & 0 & \cdots & \binom{n+2}{n+1} \end{vmatrix} \tag{1}$$

The value of this determinant is notoriously the K number of the prolate rectangle in question, viz.

$$D^{\mathrm{i}} = \binom{n+2}{n+1}^{m-1} = (n+2)^{m-1} = K\{\mathrm{R}^{\mathrm{i}}(m-1,\ n+1)\} \tag{2}$$

APPLICATION TO OBLATE RECTANGLES

General

The generation of $\mathrm{R}^{\mathrm{j}}(m,n)$ from $\mathrm{R}^{\mathrm{i}}(m-1,\ n+1)$ according to Fig. 1 is reflected in the new determinant, which emerges from D^{i} by augmenting it with a 0-th row and m-th column. A general formulation of the result is given below, where it is symbolized that D^{i} should be inserted into the $(m-1)\times(m-1)$ elements of the frame. The whole determinant has the dimension of $m\times m$.

$$K\{\mathrm{R}^{\mathrm{j}}(m,n)\} = \begin{vmatrix} \binom{n+2}{n} & \binom{n+3}{n-1} & \binom{n+4}{n-2} & \cdots & \binom{n+m}{n-m+2} & \binom{n+m}{n-m+1} \\ & & & & & \binom{n+m}{n-m+2} \\ & & & & & \binom{n+m-1}{n-m+3} \\ & & D^{\mathrm{i}} & & & \vdots \\ & & & & & \binom{n+2}{n} \end{vmatrix} \tag{3}$$

Both determinants (1) and (3) reflect the symmetry of the pertinent benzenoid in such a way that they are symmetrical around the secondary diagonal (from top-right to bottom-left).

Special Applications

The general formulation of the preceding paragraph is amenable for deducing explicit $K\{\mathrm{R}^{\mathrm{j}}(m,n)\}$ formulas, where m has (fixed) small or moderate values. The practical difficulties by expanding the determinants are the only limitations for these special applications. Below we give the results for m = 2, 3 and 4.

$$K\{\mathrm{R}^{\mathrm{j}}(2,n)\} = \begin{vmatrix} \binom{n+2}{2} & \binom{n+2}{3} \\ (n+2) & \binom{n+2}{2} \end{vmatrix} = \binom{n+2}{2}^2 - (n+2)\binom{n+2}{3} \tag{4}$$

$$K\{\mathrm{R}^{\mathrm{j}}(3,n)\} = \begin{vmatrix} \binom{n+2}{2} & \binom{n+3}{4} & \binom{n+3}{5} \\ (n+2) & \binom{n+3}{3} & \binom{n+3}{4} \\ 0 & (n+2) & \binom{n+2}{2} \end{vmatrix}$$

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

$$K\{R^j(4,n)\} = \begin{vmatrix} \binom{n+2}{2} & \binom{n+3}{4} & \binom{n+4}{6} & \binom{n+4}{7} \\ (n+2) & \binom{n+3}{3} & \binom{n+4}{5} & \binom{n+4}{6} \\ 0 & (n+2) & \binom{n+3}{3} & \binom{n+3}{4} \\ 0 & 0 & (n+2) & \binom{n+2}{2} \end{vmatrix}$$

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

$$- (n+2)\binom{n+2}{2}^2\binom{n+4}{5} \qquad (6)$$

For the sake of clarity we include an illustrative example for the last case with m=4. Fig. 3 shows the wetting and catchment areas depicted for n=3. They are surrounded by heavy lines. Fig. 4 shows the subgraphs pertaining to W_{ij} for the same example. They are represented as black

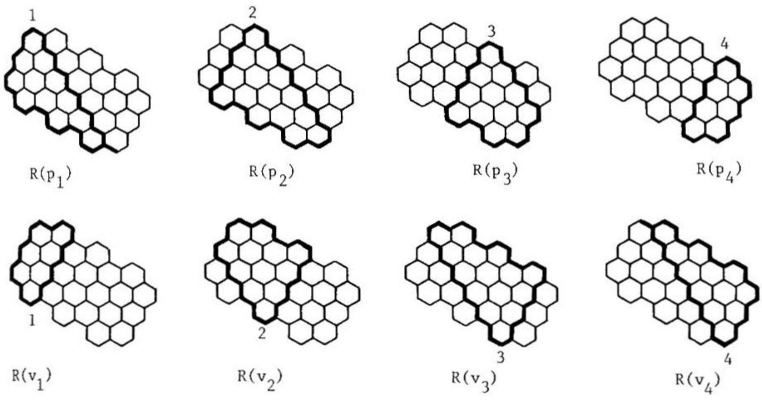

Fig. 3. Wetting areas, R(p_i), and catchment areas, R(v_j), in $R^j(m,n)$ for m=4 and n=3.

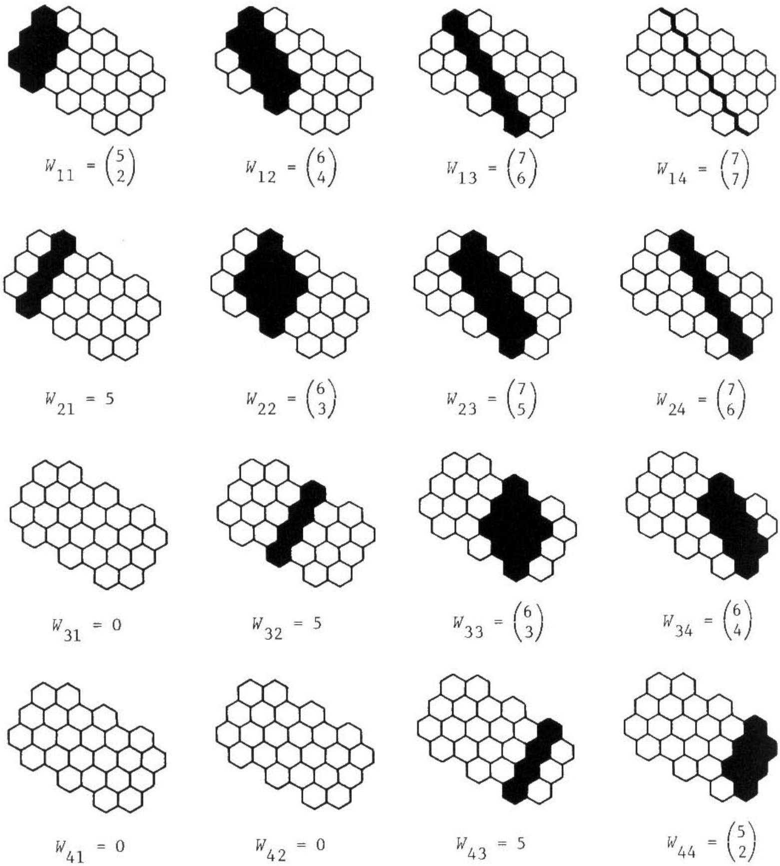

Fig. 4. Subgraphs (black hexagons and heavy lines) pertaining to W_{ij} in $R^j(m,n)$ for m=4 and n=3.

silhouettes and heavy lines on the background of the original rectangle.

The expressions (4)-(6) are equivalent to the polynomial forms, which are summarized (with appropriate references) in Ref. [5].

Linear Factors

It was conjectured[5] and later proved[7] that the polynomial $K\{R^j(m,n)\}$ for $m > 1$ has the factors $(n+1)(n+2)^m(n+3)$. This property is almost evident from the determinant form of this polynomial; cf. eqns. (3) and (1).

The first row of the determinant has the factors $(n+1)(n+2)$. The j-th row has the factor $(n+2)$ for $j = 2, 3, \ldots, m$. Furthermore, the sum of the $(m-1)$-th and m-th column has the factor $(n+3)$. Hence the above statement is proved.

APPLICATION TO INCOMPLETE OBLATE RECTANGLES

The auxiliary benzenoid classes $B(n, 2m-2, t)$, where $-n \leq t \leq n$, have been defined in previous parts of this series [5, 7, 8, 11]. We adher to the notation [11]

$$R_n^{(t)}(m) = K\{B(n, 2m-2, t)\} \qquad (7)$$

for the pertinent number of Kekulé structures.

For $0 < l < n$ the benzenoid $B(n, 2m-2, l)$ may be described as an incomplete oblate rectangle $R^j(m,n)$, where the top row holds l hexagons instead of n; cf. Fig. 5. For $l=n$ the rectangle becomes "complete": $B(n, 2m-2, n) = R^j(m,n)$.

The present method is effective for an application to $B(n, 2m-2, l)$ with the orientation shown in Fig. 5. The result is similar to eqn. (3); in fact the only difference is found in the first row of the determinant, where n is substituted by l:

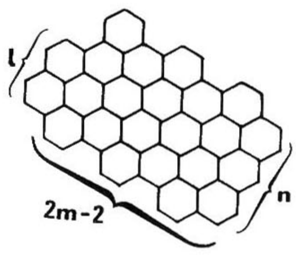

Fig. 5. The incomplete oblate rectangle, $B(n, 2m-2, l)$, suitably oriented for the application of the present method.

$$R_n^{(l)}(m) = \begin{vmatrix} \binom{l+2}{l} & \binom{l+3}{l-1} & \binom{l+4}{l-2} & \cdots & \binom{l+m}{l-m+2} & \binom{l+m}{l-m+1} \\ & & & & & \binom{n+m}{n-m+2} \\ & & & & & \binom{n+m-1}{n-m+3} \\ & & D^{i} & & & \vdots \\ & & & & & \binom{n+2}{n} \end{vmatrix} \qquad (8)$$

The elements in D^{i} are given by eqn. (1).

Special applications of (8) for $m = 2$, 3 and 4 give:

$$R_n^{(l)}(2) = \binom{n+2}{2}\binom{l+2}{2} - (n+2)\binom{l+2}{3} \qquad (9)$$

$$R_n^{(l)}(3) = \left[\binom{n+2}{2}\binom{n+3}{3} - (n+2)\binom{n+3}{4}\right]\binom{l+2}{2} - (n+2)\binom{n+2}{2}\binom{l+3}{4} + (n+2)^2\binom{l+3}{5} \qquad (10)$$

$$R_n^{(l)}(4) = \left\{\binom{n+3}{3}\left[\binom{n+2}{2}\binom{n+3}{3} - (n+2)\binom{n+3}{4}\right] - (n+2)\binom{n+2}{2}\binom{n+4}{5}\right\}\binom{l+2}{2} - (n+2)\left[\binom{n+2}{2}\binom{n+3}{3} - (n+2)\binom{n+3}{4}\right]\binom{l+3}{4} + (n+2)^2\binom{n+2}{2}\binom{l+4}{6} - (n+2)^3\binom{l+4}{7} \qquad (11)$$

For $l=n$ eqns. (9), (10) and (11) coincide with (4), (5) and (6), respectively.

For $l=0$ the incomplete oblate rectangle reduces to a certain benzenoid, B(n, $2m-2$, 0). Figure 6 shows the three cases for $m = 2$, 3 and 4. These benzenoids belong to 2-tier, 4-tier and 6-tier regular strips [4, 12], respectively. Figure 6 includes the appropriate notations for the classes in question, a parallelogram (L), pentagon (D) and tower (H). Introduce the abbreviated notation:

$B(n,2,0) = L(2,n)$ $B(n,4,0) = D(2,3,n)$ $B(n,6,0) = H_{14}(3,4,n)$

Fig. 6. Members of the classes $B(n,\ 2m-2,\ l)$ for $l=0$ and $m = 2$, 3 and 4.

$$L = K\{L(2,n)\} = R_n^{(0)}(2) \tag{12}$$

$$D = K\{D(2,3,n)\} = R_n^{(0)}(3) \tag{13}$$

$$H = K\{H_{14}(3,4,n)\} = R_n^{(0)}(4) \tag{14}$$

With these symbols eqns. (9)-(11) reduce to:

$$R_n^{(l)}(2) = L\binom{l+2}{2} - (n+2)\binom{l+2}{3} \tag{15}$$

$$R_n^{(l)}(3) = D\binom{l+2}{2} - (n+2)L\binom{l+3}{4} + (n+2)^2\binom{l+3}{5} \tag{16}$$

$$R_n^{(l)}(4) = H\binom{l+2}{2} - (n+2)D\binom{l+3}{4} + (n+2)^2L\binom{l+4}{6} - (n+2)^3\binom{l+4}{7} \tag{17}$$

APPLICATION TO ASSOCIATES TO INCOMPLETE OBLATE RECTANGLES

In eqn. (7) allowance is made for negative integer values of t; cf. the cited references [5, 7, 8, 11]. The class $B(n,\ 2m-2,\ -l)$ is referred to as associate to $B(n,\ 2m-2,\ l)$. By means of the connection

$$R_n^{(-l)}(m) = R_n^{(l)}(m) - R_n^{(l-1)}(m) \tag{18}$$

one easily obtains the determinant form of $R_n^{(-l)}(m) = K\{B(n,\ 2m-2,\ -l)\}$. It is identical to (8) part from the first row:

$$R_n^{(-l)}(m) = \left|\begin{array}{cccccc} \binom{l+1}{l} & \binom{l+2}{l-1} & \binom{l+3}{l-2} & \cdots & \binom{l+m-1}{l-m+2} & \binom{l+m-1}{l-m+1} \\ & & & & & \binom{n+m}{n-m+2} \\ & & & & & \binom{n+m-1}{n-m+3} \\ & & D^{i} & & & \cdot \\ & & & & & \cdot \\ & & & & & \cdot \\ & & & & & \cdot \\ & & & & & \binom{n+2}{n} \end{array}\right| \qquad (19)$$

The special applications to m = 2, 3 and 4 give formulas similar to (9), (10) and (11), respectively. In the form of (15)-(17) they read:

$$R_n^{(-l)}(2) = L\ (l+1) - (n+2)\binom{l+1}{2} \qquad (20)$$

$$R_n^{(-l)}(3) = D\ (l+1) - (n+2)L\binom{l+2}{3} + (n+2)^2\binom{l+2}{4} \qquad (21)$$

$$R_n^{(-l)}(4) = H\ (l+1) - (n+2)D\binom{l+2}{3} + (n+2)^2L\binom{l+3}{5} - (n+2)^3\binom{l+3}{6} \qquad (22)$$

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