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ON THE NUMBER OF KEKULÉ STRUCTURES FOR RECTANGLE-SHAPED BENZENOIDS - PART VI

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Abstract - Numbers of Kekulé structures (*K*) for oblate rectangles and related benzenoid classes are studied. The determinant formulas, based on John-Sachs theorem and presented in PART V, are expanded in terms of summations, which are convenient for practical applications. The virtue of the present methods is demonstrated by deriving the combinatorial *K* formula for the 15-tier oblate rectangle. It is a polynomial of 22-th degree.

<u>Introduction</u>. This is a continuation of the studies of the number of Kekulé structures (*K*) of oblate rectangles, $R^j(m,n)$, and related benzenoids. We adhere to the definitions and the notation introduced in the previous parts of this article series.[1]

During these studies many challenging problems have been encountered, and different methods have been devised in order to solve them.

Gutman[2] attacked the problem of deriving $K\{R^j(m,n)\}$ for some fixed values of n. He solved this task for n=1 and n=2 by introducing auxiliary benzenoid classes and treating systems of linearly coupled recurrence relations. These methods have been systematized and applied to oblate rectangles with n = 3, 4, 5 and related benzenoid classes in PART IA, PART III and elsewhere.[3-5]

Another line of these studies concerns $K\{R^j(m,n)\}$ with fixed values of m. For m=2 and m=3 the combinatorial formulas were derived already in the classical work of Gordon and Davison,[6] and also later by different methods.[7-10] In order to solve the problem for m=4 a refined application of auxiliary benzenoid classes was devised in PART IA; in this work the method of fragmentation due to Randić[11] was employed and supported by analytical computations. The fully computerized method, which actually is a numerical polynomial fitting procedure, was first applied to oblate rectangles: in

PART IA for $m=4$, in PART IIA for $m=5$, and in PART IB for $m=6$. The problem was solved for $m=7$ in PART IIB by means of a summation method.

In PART V the oblate rectangles and some auxiliary benzenoid classes are treated by a new method[12] invoking the John-Sachs theorem.[13] Combinatorial K formulas are obtained in terms of determinants, whose elements are binomial coefficients.

In the present work we pursue the developments of PART V. General formulations for the expanded determinants are given. The method is used to derive the combinatorial formula for $K\{R^j(8,n)\}$, which is a polynomial of 22-th degree in n.

Results and Discussion. In PART V a determinant for $R_n^{(l)}(m) = K\{B(n, 2m-2, l)\}$ is expanded for $0 \leq l \leq n$ and $m = 2, 3, 4$; cf. eqns. (9), (10) and (11) therein. The equations display a characteristic pattern, which obviously may be generalized for all $m \geq 2$:

$$R_n^{(l)}(m) = (-1)^{m-1}(n+2)^{m-1}\binom{l+m}{l-m+1} + \sum_{i=0}^{m-2}(-1)^i(n+2)^i R_n^{(0)}(m-i)\binom{l+i+2}{l-i} \quad (1)$$

The formula is applicable to the degenerate case of $m=1$ if the summation is omitted in that case. Then the first (external) term gives correctly $R_n^{(l)}(1) = l+1$ (cf. PART III).

A similar formula holds for $R_n^{(-l)}(m) = K\{B(n, 2m-2, -l)\}$; $0 \leq l \leq n$. A generalization of eqns. (20), (21), (22) in PART V yields

$$R_n^{(-l)}(m) = (-1)^{m-1}(n+2)^{m-1}\binom{l+m-1}{l-m+1} + \sum_{i=0}^{m-2}(-1)^i(n+2)^i R_n^{(0)}(m-i)\binom{l+i+1}{l-i} \quad (2)$$

Again the formula is applicable to $m=1$ if the summation is omitted in that case. Then the first term gives correctly $R_n^{(-l)}(1) = 1$ (cf. PART III).

In eqns. (1) and (2), if m is large enough ($m > l+2$), there will be at least one vanishing binomial coefficient in the summations. More precisely, the terms for $i > l$ all vanish. The external term vanishes for $m > l+1$. Because of this feature the practical applications of these equations may be simplified.

Here we are especially interested in $R_n(m) = R_n^{(n)}(m) = K\{R^j(m,n)\}$. On inserting $l=n$, eqn. (1) gives

$$R_n(m) = (-1)^{m-1}(n+2)^{m-1}\binom{n+m}{n-m+1} + \sum_{i=0}^{m-2} (-1)^i (n+2)^i R_n^{(0)}(m-i)\binom{n+i+2}{n-i} \qquad (3)$$

The usefulness of eqn. (3) depends on the accessibility of $R_n^{(0)}(m)$ for different values of m. The expansion of the determinant for $R_n^{(l)}(m)$ when l=0 gives (cf. PART V) for $m \geq 3$:

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

Also eqns. (3) and (4) are convenient in practical applications because of the possible occurence of vanishing binomial coefficients. If m is large enough, all terms for $i > n$ in the summation vanish. The external term vanishes when $m > n+1$ in (3) and $m > n+2$ in (4).

Eqn. (4) is a recurrence relation for $R_n^{(0)}(m)$, which gives the formulas for different m values successively in the following way. First we have as an initial condition (m=2):

$$R_n^{(0)}(2) = \binom{n+2}{2} \qquad \text{or} \qquad L = \binom{n+2}{2} \qquad (5)$$

The result is consistent with the external term of eqn. (4) when the summation is omitted. It follows

$$R_n^{(0)}(3) = R_n^{(0)}(2)\binom{n+3}{3} - (n+2)\binom{n+3}{4} \qquad \text{or} \qquad D = L\binom{n+3}{3} - (n+2)\binom{n+3}{4} \qquad (6)$$

The next step yields for $H = R_n^{(0)}(4)$:

$$H = D\binom{n+3}{3} - (n+2)L\binom{n+4}{5} + (n+2)^2\binom{n+4}{6} \qquad (7)$$

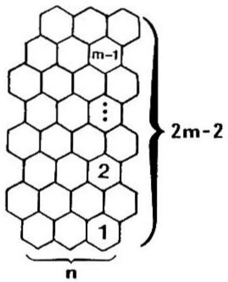
We give one more step in order that the pattern should be clear. For $G = R_n^{(0)}(5)$:

$$G = H\binom{n+3}{3} - (n+2)D\binom{n+4}{5} + (n+2)^2 L\binom{n+5}{7} - (n+3)^3\binom{n+5}{8} \qquad (8)$$

This method of successive derivation was used to develop the formulas for $R_n^{(0)}(m)$ up to m=8. The results were transferred to polynomials of n, which are collected in CHART I. The chart is supplemented with the trivial case of m=1.

CHART I. Members of B$(n,\ 2m-2,\ 0)$ with fixed values of m

B$(n,\ 2m-2,\ 0)$



$$R_n^{(0)}(1) = K\{\mathrm{B}(n,0,0)\} = 1$$

$$R_n^{(0)}(2) = K\{\mathrm{B}(n,2,0)\} = \frac{1}{2}(n+1)(n+2)$$

$$R_n^{(0)}(3) = K\{\mathrm{B}(n,4,0)\} = \frac{1}{24}(n+1)(n+2)^3(n+3)$$

$$R_n^{(0)}(4) = K\{\mathrm{B}(n,6,0)\} = \frac{1}{240}(n+1)(n+2)^4(n+3)(n^2 + 4n + 5)$$

$$R_n^{(0)}(5) = K\{\mathrm{B}(n,8,0)\} = \frac{1}{40320}(n+1)(n+2)^5(n+3)(17n^4 + 136n^3 + 439n^2 + 668n + 420)$$

$$R_n^{(0)}(6) = K\{\mathrm{B}(n,10,0)\} = \frac{1}{725760}(n+1)(n+2)^6(n+3)(31n^6 + 372n^5 + 1942n^4 + 5616n^3 + 9511n^2 + 8988n + 3780)$$

$$R_n^{(0)}(7) = K\{\mathrm{B}(n,12,0)\} = \frac{1}{159667200}(n+1)(n+2)^7(n+3)(691n^8 + 11056n^7 + 79788n^6 + 338320n^5 + 921759n^4 + 1654264n^3 + 1915562n^2 + 1315560n + 415800)$$

$$R_n^{(0)}(8) = K\{\mathrm{B}(n,14,0)\} = \frac{1}{12454041600}(n+1)(n+2)^8(n+3)(5461n^{10} + 109220n^9 + 1006407n^8 + 5617392n^7 + 21022809n^6 + 55133100n^5 + 102705053n^4 + 134421928n^3 + 118632870n^2 + 64047960n + 16216200)$$

Now eqn. (3) is practically applicable. For m = 2, 3, 4, 5 it gives the following expressions, where the symbols L, D, H and G are applied in consistence with eqns. (5)-(8).

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

$$R_n(3) = D\binom{n+2}{2} - (n+2)L\binom{n+3}{4} + (n+2)^2\binom{n+3}{5} \tag{10}$$

$$R_n(4) = H\binom{n+2}{2} - (n+2)D\binom{n+3}{4} + (n+2)^2L\binom{n+4}{6} - (n+2)^3\binom{n+4}{7} \tag{11}$$

$$R_n(5) = G\binom{n+2}{2} - (n+2)H\binom{n+3}{4} + (n+2)^2D\binom{n+4}{6} - (n+2)^3L\binom{n+5}{8} + (n+2)^4\binom{n+5}{9} \tag{12}$$

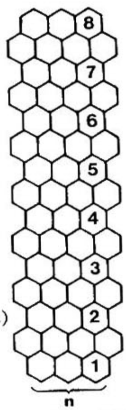
It is believed that the procedure indicated by eqns. (9)-(12) represents the so far easiest way which has been detected, to obtain combinatorial formulas for $R_n(m) = K\{\mathrm{R}^j(m,n)\}$ with fixed values of m. Other methods have been used to derive $R_n(m)$ for m up to 7 (see above).

We point out that a misprint is present in the polynomial $P_6(m) = K\{\mathrm{R}^j(6,n)\}$ in PART IB: the constant before n^5 should read 338320 (not 33820).

In CHART II we show the result obtained for $R_n(8)$ in the present work.

CHART II. The 15-tier oblate rectangle

$$^{a}R_n(8) = K\{\mathrm{R}^j(8,n)\} = \frac{1}{10461394944000}(n+1)(n+2)^8(n+3)(929569n^{12} + 22309656n^{11} + 250158485n^{10} + 1731086820n^9 + 8229767127n^8 + 28315930608n^7 + 72322500575n^6 + 138258580980n^5 + 196559445604n^4 + 203012336736n^3 + 144957849840n^2 + 64500408000n + 13621608000)$$



$\mathrm{R}^j(8,n)$

[a] The numerical factor in front of the polynomial is $\frac{1}{5!\cdot 14!}$

The formula of CHART II is of course quite impractical for hand calculations because of the large integers involved. However, the fact that it could be derived demonstrates the virtue of the present method.

Because of the untractable integers of the formula in CHART II we also give the last intermediate step in the derivation, where the numbers of digits of the integers do not exceed ten.

$$K\{R^j(8,n)\} = \frac{1}{8\cdot 13!}(n+1)(n+2)^8(n+3)[1939n^{12} + 53580n^{11} + 691553n^{10} + 5453576n^9 + 29131719n^8 + 110866764n^7 + 308164547n^6 + 630633504n^5 + 943640482n^4 + 1007609536n^3 + 729178560n^2 + 321056640n + 64864800 + \frac{1}{210}(522379n^{12} + 11057856n^{11} + 104932355n^{10} + 585835860n^9 + 2112106137n^8 + 5033910168n^7 + 7607945705n^6 + 5825545140n^5 - 1605055616n^4 - 8585665824n^3 - 8169647760n^2 - 2921486400n)] \quad (13)$$

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