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

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Abstract - The studies of the number of Kekulé structures for oblate rectangles and their auxiliary classes are continued. The new developments have led to an extension (to n=6) of the set of recurrence relations discussed in PART III.

1. INTRODUCTION

The studies of Kekulé structure counts (K) for oblate rectangle-shaped benzenoids (or simply oblate rectangles) have met with relatively difficult, and therefore challenging problems. These studies have led to the developments of several new methods. Two article series with practically the same titles were started independently by Cyvin et al. and by Chen, not anticipating the present collaboration between the authors. The two series are now combined into one as shown in the list of references.[1]

In the present paper we use the same notation as in PART III.[1] Especially the following abbreviation was introduced for the number of Kekulé structures of oblate rectangles.

$$R_n(m) = K\{\mathrm{R}^{\mathrm{j}}(m,n)\} \quad (1)$$

The K numbers for a set of auxiliary classes are given by

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

for $t = 0, \pm 1, \pm 2, \ldots, \pm n$. In particular, $R_n^{(n)}(m) = R_n(m)$. In the symbols $R_n^{(l)}(m)$ and $R_n^{(-l)}(m)$ the parameter l is defined as positive or zero.

2. COMBINATORIAL K FORMULAS FOR B(n, $2m-2$, $-l$); $m=2$ AND $m=3$

$m=2$

A formula for $K\{B(n, 2, -l)\} = R_n^{(-l)}(2)$ was given by Chen (PART IB and PART IIB)[1] as

$$R_n^{(-l)}(2) = \frac{1}{2}(n+2)(l+1)(n-l+1) \tag{3}$$

It may be written in what we shall refer to as the first representation (PART IA)[1]

$$R_n^{(-l)}(2) = \binom{n+2}{2}(l+1) - (n+2)\binom{l+1}{2} \tag{4}$$

The following form we shall refer to as the second representation.

$$R_n^{(-l)}(2) = \binom{n+2}{2}(n-l+1) - (n+2)\binom{n-l+1}{2} \tag{5}$$

The member of this class for $l=0$ and $l=n$ is the L(2,n) parallelogram in both cases. On inserting $l=0$ and $l=n$ in (4) and (5), respectively, one finds immediately as expected

$$R_n^{(0)}(2) = R_n^{(-n)}(2) = \binom{n+2}{2} \tag{6}$$

$m=3$

In order to derive $K\{B(n, 4, -l)\} = R_n^{(-l)}(3)$ we start with a special case of Chen's formula (1) of PART IB,[1] ($m=4$, $s=2$), viz.

$$R_n^{(-l)}(3) = \sum_{i=0}^{l}(n-l+1)(i+1)R_n^{(-i)}(2) + \sum_{j=l+1}^{n}(n-j+1)(l+1)R_n^{(-j)}(2) \tag{7}$$

Insert $R_n^{(-i)}(2)$ and $R_n^{(-j)}(2)$ from the first (4) and second representation (5), respectively;

$$R_n^{(-l)}(3) = (n-l+1)\sum_{i=0}^{l}(i+1)\left[(i+1)\binom{n+2}{2} - (n+2)\binom{i+1}{2}\right]$$

$$+ (l+1)\sum_{j=l+1}^{n}(n-j+1)\left[(n-j+1)\binom{n+2}{2} - (n+2)\binom{n-j+1}{2}\right] \qquad (8)$$

In the last summation we substitute j by $j = n-i$ and take the terms in reverse order. Consequently:

$$R_n^{(-l)}(3) = (n-l+1)\sum_{i=0}^{l}(i+1)\left[(i+1)\binom{n+2}{2} - (n+2)\binom{i+1}{2}\right]$$

$$+ (l+1)\sum_{i=0}^{n-l-1}(i+1)\left[(i+1)\binom{n+2}{2} - (n+2)\binom{i+1}{2}\right] \qquad (9)$$

The result is consistent with the symmetry property $K\{B(n, 2, -i)\} = K\{B(n, 2, i-n)\}$. The two summands in (9) have identical forms. They are in principle easily executed. Here we make use of the identities

$$(i+1)^2 = 2\binom{i+2}{2} - (i+1) \qquad (10)$$

$$(i+1)\binom{i+1}{2} = 3\binom{i+3}{3} - 4\binom{i+2}{2} + (i+1) \qquad (11)$$

Consequently the essential parts of the summations are readily obtained as:

$$\sum_{i=0}^{r}(i+1)^2 = 2\binom{r+3}{3} - \binom{r+2}{2} \qquad (12)$$

$$\sum_{i=0}^{r}(i+1)\binom{i+1}{2} = 3\binom{r+4}{4} - 4\binom{r+3}{3} + \binom{r+2}{2} \qquad (13)$$

where we have to use $r=l$ and $r = n-l-1$, respectively, in the two summations of (9). Eqn. (9) was consequently rendered into the form

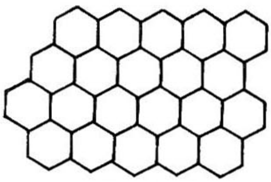
$$R_n^{(-l)}(3) = (n-l+1)\left\{ 2\left[\binom{n+3}{2} + n+2\right]\binom{l+3}{3} - \binom{n+3}{2}\binom{l+2}{2} - 3(n+2)\binom{l+4}{4} \right\}$$

$$- (l+1) \left\{ 2\left[\binom{n+3}{2} + n+2\right]\binom{n-l+2}{3} - \binom{n+3}{2}\binom{n-l+1}{2} - 3(n+2)\binom{n-l+3}{4} \right\} \tag{14}$$

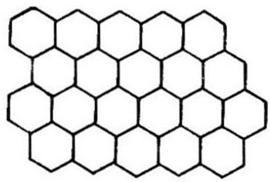
Inserting of $l=0$ and $l=n$ into (14) should both give

$$R_n^{(0)}(3) = R_n^{(-n)}(3) = \frac{1}{4}(n+2)^2\binom{n+3}{3} \tag{15}$$

which is the K formula for the four-tier pentagon.[2] The system is depicted below in the two orientations pertaining to $l=0$ and $l=n$.



B(n, 4, 0)



B(n, 4, $-n$)

In this example $n=5$ and $R_5^{(0)}(3) = R_5^{(-5)}(3) = 686$. The inserting of $l=n$ into (14) is quite manageable. One obtains

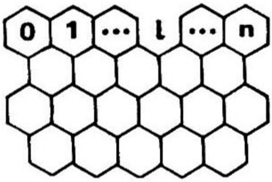
$$R_n^{(-n)}(3) = 2\left[\binom{n+3}{2} + n+2\right]\binom{n+3}{3} - \binom{n+3}{2}\binom{n+2}{2} - 3(n+2)\binom{n+4}{4} \tag{16}$$

which indeed may be reduced to the form (15).

The whole equation (14) is somewhat simplified on expanding the binomial coefficients. It was arrived at:

$$R_n^{(-l)}(3) = \frac{1}{24}(n+2)(l+1)(n-l+1)[(n-l)(n-l+2)(n + 3l + 11) + (l+2)(l+3)(4n - 3l + 8) - 6(n+2)(n+3)] \tag{17}$$

Below we give an example of a member of this class. The figure pertains to $n=5$, $l=3$; in this case $R_5^{(-3)}(3) = R_5^{(-2)}(3) = 1519$.



B(n, 4, $-l$)

A possible application of eqn. (14) or (17) would be a direct expansion of $R_n(4)$ according to PART IA:[1]

$$R_n(4) = \sum_{i=0}^{n} R_n^{(-i)}(3) R_n^{(-i)}(2) \tag{18}$$

Also the K formula for the next member (m=5) could be obtained directly by

$$R_n(5) = \sum_{i=0}^{n} [R_n^{(-i)}(3)]^2 \tag{19}$$

The expansion of the summations (18) and (19), although elementary, would be extremely tedious. We have not performed this task since the answers are already known (PART IA, PART IIA),[1] and we do not claim that the method would lead to the goal easier.

2. RECURRENCE RELATIONS FOR $R_n^{(t)}(m)$

Introduction

The auxiliary class B(n, $2m$-2, $-j'$), where $j' = [n/2]$, is of a special interest for the recurrence relations which are treated in details in PART III.[1] Below we summarize the known results so far with regard to these recurrence relations.

n	Recurrence relation
1	[a]$R_1(m+1) = 3R_1(m)$
2	[a]$R_2(m+1) = 8R_2(m) - 8R_2(m-1)$
3	[b,c]$R_3(m+1) = 15R_3(m) - 25R_3(m-1)$
4	[c,d]$R_4(m+1) = 27R_4(m) - 108R_4(m-1) + 108R_4(m-2)$
5	[e]$R_5(m+1) = 42R_5(m) - 245R_5(m-1) + 343R_5(m-2)$

[a]I. Gutman, Match 17, 3 (1985)
[b]R. Chen, J. Xinjiang Univ. 3(2), 13 (1986)
[c]S.J. Cyvin, B.N. Cyvin and J.L. Bergan, Match 19, 189 (1986) - PART IA
[d]L.X. Su, Match 20, 229 (1986)
[e]R. Chen, S.J. Cyvin and B.N. Cyvin, Match - PART III

We shall adhere to the form of eqn. (51) in PART III,[1] which defines the coefficients c_j of the recurrence relations in question. The given form applies to any classes $R_n^{(t)}(m)$. When applied to $t = -j'$ one obtains

$$R_n^{(-j')}(m+1) = \sum_{j=0}^{j'} c_j R_n^{(-j')}(m-j); \qquad j' = \left[\frac{n}{2}\right] \tag{20}$$

Nontrivial values of n, viz. $n = 1, 2, 3, \ldots$, are assumed.

Conjecture A in PART III[1] states

$$c_0 = R_n^{(-j')}(2) \tag{21}$$

Furthermore, we know from PART III[1] that, for arbitrary n,

$$R_n^{(-j')}(1) = 1 \tag{22}$$

For arbitrary $n > 1$:

$$R_n^{(-j')}(0) = 0 \tag{23}$$

In the remainder of this section we assume $n > 1$.

Preliminary derivations

Eqn. (20) applied to m=1 gives

$$R_n^{(-j')}(2) = c_0 R_n^{(-j')}(1) + \sum_{j=1}^{j'} c_j R_n^{(-j')}(1-j) = c_0 + \sum_{j=1}^{j'} c_j R_n^{(-j')}(1-j) \tag{24}$$

For n=2 and n=3 (in both cases j' = 1), the summation in (24) reduces to one term, which vanishes. Hence the result confirms Conjecture A in these special cases. For n=4 and n=5 (in both cases j' = 2), the summation acquires two terms:

$$R_4^{(-2)}(2) = c_0 + c_1 R_4^{(-2)}(0) + c_2 R_4^{(-2)}(-1) \tag{25}$$

$$R_5^{(-2)}(2) = c_0 + c_1 R_5^{(-2)}(0) + c_2 R_5^{(-2)}(-1) \tag{26}$$

By virtue of Conjecture A , together with (23) one obtains

$$R_4^{(-2)}(-1) = 0, \qquad R_5^{(-2)}(-1) = 0 \tag{27}$$

In continuation of this analysis eqn. (24) applied to n=6 (j' = 3) yields

$$R_6^{(-3)}(2) = c_0 + c_1 R_5^{(-3)}(0) + c_2 R_5^{(-3)}(-1) + c_3 R_5^{(-3)}(-2) \tag{28}$$

By the same reasoning as above one obtains that the sum of the two last terms in (28) should vanish. It seems to be a reasonable assumption, and will be verified in the following, that these two terms vanish individually, viz.

$$R_6^{(-3)}(-1) = R_6^{(-3)}(-2) = 0 \tag{29}$$

In general, provided that Conjecture A (21) is valid, one obtains by means of (23) and (24):

$$\sum_{j=2}^{j'} c_j R_n^{(-j')}(1-j) = 0 \tag{30}$$

In the following we state a supplementary conjecture, of which (29) is a special case.

Conjecture A':

$$R_n^{(-j')}(-j) = 0; \qquad j = 1, 2, \ldots., j'-1 \tag{31}$$

This conjecture states that each term in the summation (30) vanishes individually. Eqn. (27) verifies (31) for $j' = 2$ provided that (21) holds.

Corollary of Conjecture A':

$$R_n^{(-j')}(-j') = \frac{1}{c_{j'}} \tag{32}$$

Proof: Apply eqn. (20) for m=0;

$$R_n^{(-j')}(1) = \sum_{j=0}^{j'} c_j R_n^{(-j')}(-j) \tag{33}$$

or

$$1 = c_{j'} R_n^{(-j')}(-j') + \sum_{j=0}^{j'-1} c_j R_n^{(-j')}(-j) \tag{34}$$

where the summation vanishes by virtue of (23) and (31). Hence the relation (32) follows.

It is noted that we have been treating nominal values of K according to the previous definition (PART III).[1]

In the following we assume that both Conjecture A and Conjecture A' are valid.

Successive derivation of the coefficients c_j

Eqn. (20) was applied to m=0 and m=1 in (33) and (24), respectively. The process can be continued. For m=2 one obtains

$$R_n^{(-j')}(3) = c_0 R_n^{(-j')}(2) + c_1 R_n^{(-j')}(1) + \sum_{j=2}^{j'} c_j R_n^{(-j')}(2-j) \tag{35}$$

where all nonvanishing terms have been extracted from the summation, while the summation itself vanishes by virtue of (23) and (31). Hence

$$c_1 = R_n^{(-j')}(3) - c_0 R_n^{(-j')}(2) = R_n^{(-j')}(3) - [R_n^{(-j')}(2)]^2 \tag{36}$$

The next step (m=3) yields in the same way

$$c_2 = R_n^{(-j')}(4) - c_0 R_n^{(-j')}(3) - c_1 R_n^{(-j')}(2)$$

$$= R_n^{(-j')}(4) - 2R_n^{(-j')}(2) R_n^{(-j')}(3) + [R_n^{(-j')}(2)]^2 \qquad (37)$$

In general:

$$c_j = R_n^{(-j')}(j+2) - \sum_{k=0}^{j-1} c_k R_n^{(-j')}(j-k+1) \qquad (38)$$

Application to n=6

We will show an application of the above procedure to n=6. Then j' = 3, and hence we seek four coefficients in the recurrence relation, viz.

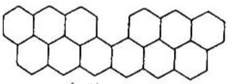
$$R_6(m+1) = c_0 R_6(m) + c_1 R_6(m-1) + c_2 R_6(m-2) + c_3 R_6(m-3) \qquad (39)$$

By means of Conjecture C (PART III),[1] which states

$$c_3 = -c_2 \qquad (n=6) \qquad (40)$$

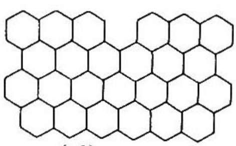
the number of unknown coefficients is reduced to three (c_0, c_1, c_2). They are obtained, in accordance with eqns. (21), (36) and (37), by means of three K numbers:

B(6, 2, -3)



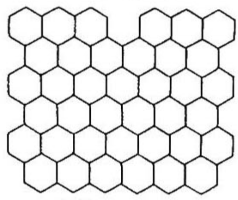
$R_6^{(-3)}(2) = 64$

B(6, 4, -3)



$R_6^{(-3)}(3) = 3456$

B(6, 6, -3)



$R_6^{(-3)}(4) = 182272$

The numerical values are found in the tables of PART III.[1]

The net result is:

$$\boxed{R_6(m+1) = 64R_6(m) - 640R_6(m-1) + 2048R_6(m-2) - 2048R_6(m-3)} \qquad (41)$$

The formula apparatus, which was used to derive the relation (41), is based on conjectures. However, the result was verified by means of a sufficient number of numerical tests. The tabulated values in PART III[1] supply sufficient material for this purpose. The correctness of the final result (41) confirms in particular the nominal values of eqn. (29).

4. EXPLICIT EXPRESSIONS OF c_j; $j=0$ AND $j=1$

We are now in the position to express c_0 and c_1 explicitly as functions of n.

Eqn. (3) applied to $l = j' = [n/2]$ gives c_0 in accord with Conjecture A (21). Explicitly:

$$c_0 = R_n^{(-j')}(2) = \begin{cases} \frac{1}{8}(n+2)^3; & n = 0, 2, 4, \ldots. \\ \frac{1}{8}(n+1)(n+2)(n+3); & n = 1, 3, 5, \ldots. \end{cases} \tag{42}$$

Here $n=0$ covers the trivial case saying that $R_0(m) = 1$ for all m.

Eqn. (17) applied to $l = j'$ gives:

$$R_n^{(-j')}(3) = \begin{cases} \frac{1}{384}(n+2)^4(5n^2 + 20n + 24); & n = 0, 2, 4, \ldots. \\ \frac{1}{384}(n+1)(n+2)^2(n+3)(5n^2 + 20n + 23); & n = 1, 3, 5, \ldots. \end{cases} \tag{43}$$

On inserting (42) and (43) into (36) the following explicit formula for c_1 was achieved.

$$c_1 = \begin{cases} -\frac{1}{384}n(n+2)^4(n+4); & n = 2, 4, 6, \ldots. \\ -\frac{1}{384}(n-1)(n+1)(n+2)^2(n+3)(n+5); & n = 3, 5, 7, \ldots. \end{cases} \tag{44}$$

5. CONCLUSION

The expressions for c_0 and c_1 as given in eqns. (42) and (44), respectively, display remarkable simple forms inasmuch as they are completely factored into linear factors. In order to test whether this regularity continues through higher values of j one should have the expressions of

$R_n^{(-l)}(4)$, $R_n^{(-l)}(5)$, etc., if it is adherred to the same procedure as above. The method used in Section 2 to derive $R_n^{(-l)}(3)$ is not amenable for extension to larger values of m. A more powerful method, based on the John-Sachs theorem,[3] was recently employed for derivations of different kinds of K formulas. This topic, as far as the rectangles and related benzenoid classes are concerned, is to be treated in the next part of this article series.

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