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NUMBER OF KEKULÉ STRUCTURES FOR RECTANGLE-SHAPED BENZENOIDS - PART II

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Abstract - The fully computerized method was applied to derive the algebraic formula for the number of Kekulé structures of Rj(5,n), the 9-tier oblate rectangular benzenoid. The result is a polynomial of 13-th degree in n.

1. INTRODUCTION

In Part I [1] a formula for $K\{\mathrm{Rj}(4,n)\}$ was derived for the first time. This means the number of Kekulé structures for the oblate 7-tier rectangular benzenoid. The result turned out to be a polynomial of 10-th degree in n. The bibliography of the cited paper [1] should be consulted for a broader context of the present type of work. Furthermore, a number of useful reviews [2-6] have appeared. At the end of Paper I [1] a method referred to as fully computerized is outlined. In the present work this method was applied to Rj(5,n), the 9-tier oblate rectangle.

The final formula of $K\{\mathrm{Rj}(5,n)\}$ in the form of a 13-th degree polynomial is shown in CHART I.

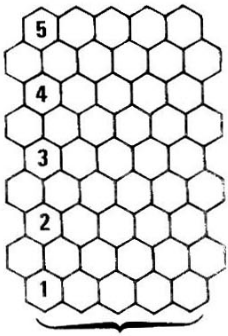
2. THE POLYNOMIAL $P_5(n)$ AND ITS DEGREE

Define

$$P_5(n) = K\{\mathrm{Rj}(5,n)\} \tag{1}$$

In the computerized method it is important to predict theoretically the degree, say d_5, of the polynomial (1). According to the basic formulas of Part I ([1], Section 6) one has

CHART I - The oblate rectangle Rj$(5,n)$.



$$K\{\mathrm{Rj}(5,n)\}$$
$$= \frac{1}{362880}(n+1)(n+2)^5(n+3)(31n^6 + 372n^5 + 1942n^4 + 5616n^3 + 9511n^2 + 8988n + 3780)$$

$$P_4(n) = \sum_{i=0}^{n} K\{\mathrm{B}(n,6,\ -i)\} \tag{2}$$

and

$$P_5(n) = \sum_{i=0}^{n} K\{\mathrm{B}(n,6,\ -i)\}\left[\binom{n+2}{2}(i+1) - (n+2)\binom{i+1}{2}\right] \tag{3}$$

We may speak about the combined degree in i and n with reference to the above summations. It is the maximum of $p+q$ for $n^p i^q$. From the degree of $P_4(n)$, which is known to be $d_4 = 10$ [1] we infer that the combined degree in the summation of eqn. (2) is 9. Consequently the combined degree in the summation (3) is 12, and (after the summation is executed) the degree of $P_5(n)$ in n becomes 13. In a simplified way we may infer directly from the bracketed factor in eqn. (3) that the degree increases 3 units from P_4 to P_5. Strictly speaking we have only proved $d_5 \leq 13$, which is sufficient for our purpose, and where the sign of equality is highly probable.

3. THE POLYNOMIAL $Q_5(n)$

As a working hypothesis assume that $P_5(n)$ is partially factorized according to [1]

$$P_5(n) = (n+1)(n+2)^5(n+3)Q_5(n) \tag{4}$$

where $Q_5(n)$ is a polynomial of 6-th degree in n. We write this polynomial as

$$Q_5(n) = A + B\binom{n}{1} + C\binom{n}{2} + D\binom{n}{3} + E\binom{n}{4} + F\binom{n}{5} + G\binom{n}{6} \tag{5}$$

The 7 coefficients of eqn. (5) are to be determined by means of 7 numerical solutions for $K\{\mathrm{Rj}(5,n)\}$ (TABLE 1 of Part I [1]): $P_5(0) = 1$, $P_5(1) = 162$, $P_5(2) = 6336$, $P_5(3) = 111\,250$, $P_5(4) = 1\,167\,291$, $P_5(5) = 8\,557\,164$, $P_5(6) = 48\,179\,200$ (the last number, being greater than 10^7, was not entered into TABLE 1 of Part I). The scheme of computation in the shape of Pascal's triangle is given below.

$$\begin{array}{lcl}
1/96 = & A \quad ; & A = 1/96 \\
1/12 = & A + B \quad ; & B = 7/96 \\
33/80 = & A + 2B + C \quad ; & C = 41/160 \\
89/60 = & A + 3B + 3C + D \quad ; & D = 233/480 \\
14411/3360 = & A + 4B + 6C + 4D + E \quad ; & E = 853/1680 \\
297/28 = & A + 5B + 10C + 10D + 5E + F \quad ; & F = 31/112 \\
23525/1008 = & A + 6B + 15C + 20D + 15E + 6F + G ; & G = 31/504
\end{array}$$

On inserting into eqns. (4) and (5) one obtains

$$P_5(n) = \frac{(n+1)(n+2)^5(n+3)}{10080}\left[620\binom{n}{6} + 2790\binom{n}{5} + 5118\binom{n}{4} + 4893\binom{n}{3} + 2583\binom{n}{2} + 735n + 105\right] \tag{6}$$

4. DISCUSSION OF EQUATION (6)

A general validity of eqn. (6) is not ascertained because of the unproved hypothesis of eqn. (4). A verification of eqn. (6) could be achieved by a numerical test of 7 additional K values. This number of tests can be lowered if we prove eqn. (4) to be sound at least for some of the factors. In the subsequent section we demonstrate that $(n+2)^2$ is a factor in $P_5(n)$. Consequently we will have to verify eqn. (6) for 5 additional K values.

5. SOME AUXILIARY BENZENOID CLASSES

In Part I [1] the auxiliary benzenoids $B(n,4,x)$ are defined for $x = 0, \pm 1, \pm 2, \ldots, \pm n$. Furthermore, the basic relations [1] imply the following relation as an alternative to eqn. (3).

$$P_5(n) = \sum_{i=0}^{n} [K\{B(n,4,\ -i)\}]^2 \tag{7}$$

It has been found

$$K\{B(n,4,\ -l)\} = K\{B(n,4,l)\} - K\{B(n,4,\ l-1)\}; \qquad l \geq 1 \tag{8}$$

while an algebraic formula for $l \geq 0$ was derived:

$$\begin{aligned} K\{B(n,4,l)\} = {} & \frac{1}{3}\binom{n+2}{2}(2l+3)\binom{l+2}{2}\left[(n+2)(l+1) - \binom{l+2}{2}\right] \\ & - \frac{1}{4}(n+2)(3l+5)\binom{l+2}{3}\left[(n+2)(l+1) + \binom{n+2}{2} - \binom{l+2}{2}\right] \\ & + \frac{1}{10}(n+2)^2\binom{l+2}{3}(3l^2+6l+1) + (n+1)\binom{n+2}{2}\binom{l+2}{2}\left[\binom{n+2}{2} - \binom{l+2}{2}\right] \\ & - (n+2)(2n+1)\binom{l+2}{2}\left[\binom{n+2}{3} - \binom{l+2}{3}\right] + 3(n+2)\binom{l+2}{2}\left[\binom{n+2}{4} - \binom{l+2}{4}\right] \end{aligned} \tag{9}$$

Here we observe the common factor $(n+2)$. The same will be present in eqn. (8), and according to eqn. (7) the $P_5(n)$ polynomial will possess the factor $(n+2)^2$.

5. SUPPLEMENTARY NUMERICAL COMPUTATIONS

Equation (9) was used to compute the K numbers for the auxiliary benzenoids $B(n,4,l)$, where $0 \leq l \leq n$, and $n = 7, 8, 9, 10, 11$. The numerical results (cf. TABLE 1) were used to obtain $K\{B(n,4,\ -l)\}$ according to eqn. (8) for the same n values, and $1 \leq l \leq n$. The resulting values (TABLE 1) were finally used to compute, according to eqn. (7), the desired 5 additional values of $P_5(n) = K\{Rj(5,n)\}$. These are the results:

$$P_5(7) = 221\,578\,092$$

$$P_5(8) = 868\,388\,125$$

$$P_5(9) = 2\,989\,428\,662$$

TABLE 1. Numbers of K for $B(n,4,x)$ with n = 7, 8, 9, 10, 11.

x \ n	7	8	9	10	11
11					522886
10				298584	507507
9			162382	288288	477763
8		83325	155727	268488	435513
7	39852	79200	143022	240624	383292
6	37422	71400	125356	206640	324142
5	32886	60725	104181	168840	261443
4	26811	48225	81191	129744	198744
3	19926	35100	58201	91944	139594
2	13041	22600	37026	57960	87373
1	6966	11925	19360	30096	45123
0	2430	4125	6655	10296	15379
-1	4536	7800	12705	19800	29744
-2	6075	10675	17666	27864	42250
-3	6885	12500	21175	33984	52221
-4	6885	13125	22990	37800	59150
-5	6075	12500	22990	39096	62699
-6	4536	10675	21175	37800	62699
-7	2430	7800	17666	33984	59150
-8		4125	12705	27864	52221
-9			6655	19800	42250
-10				10296	29744
-11					15379

$$P_5(10) = 9\ 244\ 901\ 952$$

$$P_5(11) = 26\ 126\ 403\ 238$$

These 5 additional numbers were found to fit into eqn. (6).

6. CONCLUSION

The above analysis has proved the general validity of eqn. (6) as the number of Kekulé structures for $Rj(5,n)$. The formula was transferred into the polynomial form given in CHART I.

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