match no. 21 pp. 277-284 1986

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

Chen Rong-si

College of Finance and Economics
Fuzhou University, Fuzhou, Fujian
The People's Republic of China

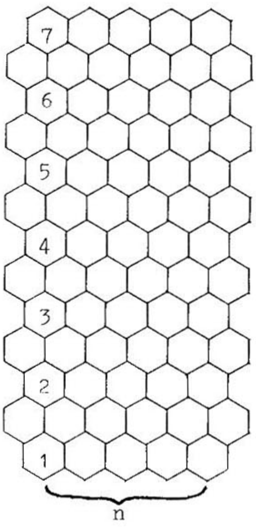
(Received: December 1986)

Abstract - A new fully computerized method (called summation method) was developed which leads to algebraic formulas for the number of Kekulé structures (K) of oblate rectangular benzenoids (Rj(m,n)). This method was applied to derive the algebraic formula for K number of Rj(7,n), the 13-tier oblate rectangular benzenoid.

1. INTRODUCTION

As mentioned in Part I [1], Cyvin et al. first developed a fully computerized method to deal with the enumeration problem of Kekulé structures of oblate rectangular benzenoids Rj(m,n). This fully computerized method is based on the important fact that the algebraic formula for K{Rj(m,n)} is a polynomial ($P_m(n)$) in powers of n with degree not greater than 3m-2 [2,3]. In using this method one can take the advantage that the polynomial $P_m(n)$ $(m \geq 2)$ has factors $n+1$, $n+3$ and $(n+2)^m$. For a wider context of the present type of work, the reader should consult the references cited in Part I (1). Furthermore, the reader can get benefit from recently published papers (4-8).

In the present work, a new type of fully computerized method referred to as summation method is outlined and is used to derive the polynomial $P_7(n)$ for Rj(7,n), viz. the 13-tier oblate rectangular benzenoid (see CHART I).



$$K\{Rj(7,n)\} = P_7(n) = \frac{1}{6227020800}(n+1)(n+2)^7(n+3)(5461n^{10}+109220n^9+1006407n^8+5617392n^7+21022809n^6+55133100n^5+102705053n^4+134421928n^3+118632870n^2+64047960n+16216200)$$

CHART I - The oblate rectangle Rj(7,n).

2. SUMMATION METHOD

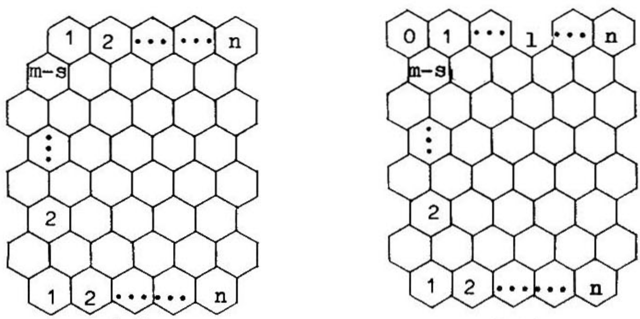
The following recurrence relations were derived for the first time in [1] .

$$K\{B(n,2(m-s),-l)\} = \sum_{i=o}^{l}(n+1-l)(i+1)K\{B(n,2(m-s-1),-i)\}$$

$$+ \sum_{i=l+1}^{n}(n+1-i)(l+1)K\{B(n,2(m-s-1),-i)\}$$

$(1 \leqslant s \leqslant m-2; l=0,1,\ldots,n)$

For the auxiliary benzenoid classes $B(n,2(m-s),-l)$, $s=1,2,\ldots,m-1$; $l=0,1,\ldots,n$, see CHART II.



l=0   l ⩾ 1

CHART II - Auxiliary benzenoid classes $B(n,2(m-s),-l)$

By applying successively the above relations to the following equation

$$K\{Rj(m,n)\} = \sum_{l=o}^{n} K\{B(n,2(m-1),-l)\}$$

one obtains (1)

$$P_m(n)=K\{Rj(m,n)\} = \sum_{i=o}^{n} d_i^{(m-1)}\ K\{B(n,2,-i)\} \qquad (1)$$

where $K\{B(n,2,-i)\} = \frac{1}{2}\ (n+2)(i+1)(n+1-i)$

and $d_i^{(s)}$ is defined by the following recurrence formulas

$$d_i^{(1)}=1$$

$$d_i^{(s)}= \sum_{j=o}^{n} d_j^{(s-1)} a_{ij} \qquad (2 \leqslant s \leqslant m-1)$$

where

$$a_{ij} = \begin{cases} (j+1)(n+1-i) & \text{if } 0 \leqslant j \leqslant i \\ (i+1)(n+1-j) & \text{if } i+1 \leqslant j \leqslant n \end{cases}$$

Thus if we denote z=n+2, then we have

$$d_i^{(s)} = \{z-(i+1)\} \sum_{j=o}^{i} \{d_j^{(s-1)}(j+1)\} + (i+1) \sum_{j=i+1}^{n} \{(z-(j+1))d_j^{(s-1)}\}$$

$$= \{z-(i+1)\} \sum_{j=o}^{i} \{d_j^{(s-1)}(j+1)\} + (i+1) \sum_{j=o}^{n} \{d_j^{(s-1)}\{z-(j+1)\}\}$$

$$-(i+1) \sum_{j=o}^{i} \{d_j^{(s-1)}\{z-(j+1)\}\}$$

$$(s=2,3,\ldots,m-1) \qquad (2)$$

Therefore, in order to obtain $P_m(n)$ for each fixed value of m, it suffices to take summations successively according to the formula (2) and finally according to (1). This method is entirely based on summation formulas and needs no numerical value of $K\{Rj(m,n)\}$. That is why it is called summation method.

3. THE SUMMATION FORMULAS $\sum_{j=1}^{n+1} j^p$ WITH FIXED VALUES OF P(≥1).

The summation method outlined in the above section needs the summation formulas $\sum_{j=1}^{n+1} j^p$, where p is a fixed natural number. By a similar reasoning as in section 5 of Part I [1], one finds the following basic formula.

$$\sum_{j=1}^{n+1} j^p = \frac{1}{p+1}\Big\{(n+1)(n+2)\sum_{i=1}^{p}\Big[\binom{p}{i}\sum_{t=0}^{i-1}\binom{i-1}{t}n^t\Big] - \sum_{i=1}^{p-1}\Big[\binom{p+1}{i}\sum_{j=1}^{n+1} j^i\Big]\Big\}$$

The first twelve formulas for $\sum_{j=1}^{n+1} j^p$ which are needed in the following section are listed in **TABLE I**.

4. THE POLYNOMIAL $P_m(n)$ FOR m=7.

In this section the summation method is used to derive the polynomial $P_7(n)$, viz. the algebraic formula for K number of Rj(7,n), the 13-tier oblate rectangular benzenoid. The result is a polynomial of 19-th degree in n and has factors $(n+1)$, $(n+2)^7$ and $(n+3)$, which is consistent with the known result about the polynomial $P_m(n)$ [1].

By using the recurrence formula (2) in section 2 and the summation foumulas listed in **TABLE I**, we obtain $d_i^{(s)}$, s=1,2, ...,6; successively. The results are listed in TABLE II. Note that $d_i^{(s)}$ $(1 \leqslant s \leqslant m-1)$ is a polynomial in n and i as mentioned in section 4 of Part I [1].

TABLE I. The summation formulas $\sum_{j=1}^{n+1} j^p$ for $1 \leqslant p \leqslant 12$.

p	$\sum_{j=1}^{n+1} j^p$
1	$1/2\ (n+1)(n+2)$
2	$1/6\ (n+1)(n+2)(2n+3)$
3	$1/4\ (n+1)^2(n+2)^2$
4	$1/30\ (n+1)(n+2)(2n+3)(3n^2+9n+5)$
5	$1/12\ (n+1)^2(n+2)^2(2n^2+6n+3)$
6	$1/42\ (n+1)(n+2)(2n+3)(3n^4+18n^3+36n^2+27n+7)$
7	$1/24\ (n+1)^2(n+2)^2(3n^4+18n^3+35n^2+24n+6)$
8	$1/90\ (n+1)(n+2)(2n+3)(5n^6+45n^5+155n^4+255n^3+209n^2+87n$ $+15)$
9	$1/20\ (n+1)^2(n+2)^2(2n^6+18n^5+61n^4+96n^3+73n^2+30n+5)$
10	$1/66\ (n+1)(n+2)(2n+3)(3n^8+36n^7+176n^6+450n^5+650n^4$ $552n^3\ +290n^2+87n+11)$
11	$1/24\ (n+1)^2(n+2)^2(2n^8+24n^7+116n^6+288n^5+395n^4+318n^3$ $+169n^2+48n+6)$
12	$1/2730\ (n+1)(n+2)(2n+3)(105n^{10}+1575n^9+9975n^8$ $+34650n^7+72310n^6+95130n^5$ $+83320n^4+51045n^3+19903n^2$ $+4359n+455)$

TABLE II . The expressions of $d_i^{(s)}$,where z=n+2, j=i+1.

s	$d_i^{(s)}$
1	1
2	$1/2\ z(zj-j^2)$
3	$1/24\ z^2\{j^4-2zj^3-j^2+z(z^2+1)j\}$
4	$1/720\ z^3\{-j^6+3zj^5+5j^4-5z(z^2+2)j^3-4j^2+z(3z^4+5z^2+4)j\}$
5	$1/40320\ z^4\{j^8-4zj^7-14j^6+14z(z^2+3)j^5+49j^4-14z(2z^4+5z^2+7)j^3 -36j^2+z(17z^6+42z^4+49z^2+36)j\}$
6	$1/3628800\ z^5\{-j^{10}+5zj^9+30j^8-30z(z^2+4)j^7-273j^6 +21z(6z^4+20z^2+39)j^5+820j^4 -5z(51z^6+168z^4+273z^2+328)j^3-576j^2 +z(155z^8+510z^6+819z^4+820z^2+576)j\}$

Finally, substitution of $d_i^{(6)}$ into formula (1) in section 2 yields

$$P_7(n)=1/7257600\ z^6\Big\{\sum_{j=1}^{n+1} j^{12} -6z\sum_{j=1}^{n+1} j^{11} +5(z^2-6)\sum_{j=1}^{n+1} j^{10}$$

$$+30z(z^2+5)\sum_{j=1}^{n+1} j^9-3(10z^4+40z^2-91)\sum_{j=1}^{n+1} j^8$$

$$-21z(6z^4+20z^2+52)\sum_{j=1}^{n+1} j^7 +(126z^6+420z^4+819z^2$$

$$-820)\sum_{j=1}^{n+1} j^6 +5z(51z^6+168z^4+273z^2+492)\sum_{j=1}^{n+1} j^5$$

$$-(255z^8+840z^6+1365z^4+1640z^2-576)\sum_{j=1}^{n+1} j^4$$

$$-z(155z^8+510z^6+819z^4+820z^2+1152)\sum_{j=1}^{n+1} j^3$$

$$+z^2(155z^8+510z^6+819z^4+820z^2+576)\sum_{j=1}^{n+1} j^2\}$$

After inserting of the summation formulas given in TABLE I, it can be reduced to the polynomial as shown in CHART I.

REFERENCES

1 Chen Rong-si,MATCH,submitted.

2 S.J.Cyvin,B.N.Cyvin and J.L.Bergan,MATCH 19,189 (1986).

3 S.J.Cyvin,Match 19,213 (1986).

4 S.J.Cyvin and I.Gutman,Comp. & Maths. with Appls. 12B, 859 (1986).

5 S.J.Cyvin,Monatsh. Chem. 117,33 (1986).

6 S.J.Cyvin,B.N.Cyvin and I.Gutman,Z. Naturforsch. 40a, 1253 (1985).

7 S.J.Cyvin and I.Gutman,Z.Naturforsch. 41a,1079 (1986).

8 I.Gutman and S.J.Cyvin,J.Molecular Structure (Theochem), 325,138 (1986).