THE NUMBER OF KEKULÉ STRUCTURES FOR RECTANGLE-SHAPED BENZENOIDS: PART VII

CHEN Rong-si^a and S. J. CYVIN

^aSchool of Mathematics, Georgia Institute of Technology, Atlanta, GA 30332, USA; on leave from: Fuzhou University, Fuzhou, Fujian, The People's Republic of China

bDivision of Physical Chemistry, The University of Trondheim, N-7034 Trondheim-NTH, Norway

(Received: February 1988)

Abstract: The studies of the number of Kekulé structures for oblate rectangle-shaped benzenoids are continued. A general method - the matrix method - is developed in order to obtain the recurrence relations discussed in PART III. Furthermore, a conjecture concerning the coefficients of the recurrence relations is rigorously proved.

1. INTRODUCTION

This is a continuation of the studies of the number of Kekulé structures (K) of oblate rectangles, $R^{j}(m,n)$. In PART III of this article series it was found that there exist recurrence relations for the K number of $R^{j}(m,n)$ with fixed n values. The recurrence relations for $K\{R^{j}(m,n)\}$ are given up to n=6 in PART II and PART III.

In the present paper we develop a matrix approach to the recurrence relations for $K\{\mathbb{R}^{\hat{\mathbf{J}}}(m,n)\}$. By this method direct calculations of determinants lead to the special cases of $n=2,3,\ldots,10$. There is no hindrance against an extension to still higher values of n.

2. THE MATRIX METHOD

We use the same notation as in PART III. In particular, the following abbreviations are used.

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

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

A basic formula in PART III reads:

$$R_n(m+j) = \sum_{i=0}^n R_n^{(-i)} (j+1) R_n^{(-i)} (m)$$

It yields together with the symmetry property $R_n^{\ (-i)} = R_n^{\ (i-n)}$:

$$\begin{bmatrix} R_{n}(m) \\ R_{n}(m+1) \\ \vdots \\ R_{n}(m+j^{*}) \end{bmatrix} = J_{n} \begin{bmatrix} R_{n}^{(0)}(m) \\ R_{n}^{(-1)}(m) \\ \vdots \\ R_{n}^{(-j^{*})}(m) \end{bmatrix}$$
(2.1)

where j' = [n/2], and J_n is a $(j'+1)\times(j'+1)$ square matrix with the general element equal to

$$(J_n)_{rs} = 2R_n^{(1-s)}(r)$$
 if n is odd, or if n is even and $1 \le s \le j^*$; $(J_n)_{rs} = R_n^{(1-s)}(r)$ if n is even and $s = j^* + 1$.

Therefore, when n is even

$$\mathbf{J}_n = \begin{bmatrix} 2R_n^{(0)}(1) & 2R_n^{(-1)}(1) & \dots & 2R_n^{(-j'+1)}(1) & R_n^{(-j')}(1) \\ 2R_n^{(0)}(2) & 2R_n^{(-1)}(2) & \dots & 2R_n^{(-j'+1)}(2) & R_n^{(-j')}(2) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 2R_n^{(0)}(j') & 2R_n^{(-1)}(j') & \dots & 2R_n^{(-j'+1)}(j') & R_n^{(-j')}(j') \\ 2R_n^{(0)}(j'+1) & 2R_n^{(-1)}(j'+1) & \dots & 2R_n^{(-j'+1)}(j'+1) & R_n^{(-j')}(j'+1) \end{bmatrix}$$

and when n is odd

$$\mathbf{J_n} = \begin{bmatrix} 2R_n^{(0)}(1) & 2R_n^{(-1)}(1) & \dots & 2R_n^{(-j'+1)}(1) & 2R_n^{(-j')}(1) \\ 2R_n^{(0)}(2) & 2R_n^{(-1)}(2) & \dots & 2R_n^{(-j'+1)}(2) & 2R_n^{(-j')}(2) \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 2R_n^{(0)}(j') & 2R_n^{(-1)}(j') & \dots & 2R_n^{(-j'+1)}(j') & 2R_n^{(-j')}(j') \\ 2R_n^{(0)}(j'+1) & 2R_n^{(-1)}(j'+1) & \dots & 2R_n^{(-j'+1)}(j'+1) & 2R_n^{(-j')}(j'+1) \end{bmatrix}$$

The following shows J_n for n=2, 3,, 10. Here the number above the i-th column (or on the right-hand side of the j-th row) is the common factor extracted from the i-th column (or j-th row).

$$J_{2} = \begin{bmatrix} 1 & 1 \\ 2 & 3 \end{bmatrix}_{2} \quad J_{3} = \begin{bmatrix} 1 & 1 \\ 2 & 3 \end{bmatrix}_{5} \quad J_{4} = \begin{bmatrix} 2 & 2 \\ 1 & 1 & 1 \\ 5 & 8 & 9 \\ 35 & 60 & 69 \end{bmatrix}_{3}^{3} \quad J_{5} = \begin{bmatrix} 2 & 2 & 2 \\ 1 & 1 & 1 \\ 3 & 5 & 6 \\ 14 & 25 & 31 \end{bmatrix}_{7}^{7}$$

We now express (2.1) in another form as follows.

$$\begin{bmatrix} R_{n}^{(0)}(m) \\ R_{n}^{(-1)}(m) \\ \vdots \\ R_{n}^{(-j^{+})}(m) \end{bmatrix} = J_{n}^{-1} \begin{bmatrix} R_{n}^{(m)} \\ R_{n}^{(m+1)} \\ \vdots \\ R_{n}^{(m+j^{+})} \end{bmatrix}$$
(2.2)

where J_n^{-1} is the inverse matrix of J_n .

Let $J_n(i,j)$ denote the submatrix of J_n obtained from J_n by deleting the i-th row and the j-th column. Denote

$$u(i,j) = (-1)^{i+j} \det_{n}(i,j)$$
 (2.3)

By the standard methods of matrix calculus one obtains

$$(J_n^{-1})_{ij} = u(j,i)/\det J_n$$
 Thus from (2.2) we have

$$R_n^{(0)}(m) = (1/\det_n^{-1})[u(1,1)R_n(m) + u(2,1)R_n(m+1) + \dots + u(j'+1, 1)R_n(m+j')]$$

which together with
$$R_n^{(0)}(m) = (1/2)(n+2)R_n^{(m-1)}$$

according to eqn. (21) of PART III yields

$$c_{j} = -u(j'-j, 1)/u(j'+1, 1) ; j = 0, 1, \dots, j'-1$$

$$c_{j'} = (1/2)(n+2)\det J_n/u(j'+1, 1) (2.5)$$

Therefore, when J_n is given, the recurrence relation for $R_n(m)$ is available by direct calculation of determinants. By formulas (2.5) it was arrived at

3. THE DETERMINANT OF J

From the above section one sees that the determinant J_n is the denominator of each entry of J_n^{-1} . Now we investigate the explicit formula for detJ.

In order to simplify the derivation of detd,, we want to extract some common factors from each column and row. By the definition of J_n it is not difficult to see that 2 is a common factor of each column except the (j'+1)th column in the case when n is even. Moreover, besides the factor 2, the i-th row $(i \geq 2)$ of J_n has the common factor $(n-2)^{i-1}$. This is evident for i=2 from the known formula

$$R_n^{(-t)}(2) = (1/2)(n+2)(n-t+1)(t+1)$$

Now suppose that each element of the (i-1)-th row, viz. $R_n^{(-t)}(i-1)$, has the factor $(n+2)^{i-2}$. Thus we can write $R_n^{(-t)}(i-1) = (n+2)^{i-2}f(t,n)$

$$R_n^{(-t)}(i-1) = (n+2)^{i-2} f(t,n)$$

where f(t,n) is a polynomial in t and n.

We now apply formula (1) of PART IB to the elements of the i-th row. We have

$$\begin{split} R_{n}^{\;\;(-j)}(i) &= \sum_{t=0}^{j} \; (n+1-j) \, (t+1) R_{n}^{\;\;(-t)}(i-1) \; + \sum_{r=j+1}^{n} \; (n+1-r) \, (j+1) R_{n}^{\;\;(-r)}(i-1) \\ &= \sum_{t=0}^{j} \; [\; (n+2) \; - \; (j+1) \,] \, (t+1) \, (n+2)^{i-2} f(t,n) \\ &+ \sum_{r=j+1}^{n} \; [\; (n+2) \; - \; (r+1) \,] \, (j+1) \, (n+2)^{i-2} f(r,n) \\ &= \; (n+2)^{i-1} \, \Big[\sum_{t=0}^{j} \; (t+1) f(t,n) \; + \sum_{r=j+1}^{n} \; (j+1) f(r,n) \, \Big] \\ &- \; (n+2)^{i-2} \sum_{t=0}^{n} \; (j+1) \, (t+1) f(t,n) \end{split}$$

As seen in PART IB the summation $\sum_{i=1}^{n} (t+1)$ has the factor (n+2). One can

verify that the last summation in the above formula has the factor (n+2) in a similar way as in Section 6 of PART IB. Therefore, $R_n^{(-j)}(i)$ has the factor $(n+2)^{i-1}$.

Now we are in the position to derive the explicit formula for detd. Since the cases with even and odd n behave slightly differently, we distinguish two cases.

(a) n is odd

Introduce $e_{i,j} = (1/2)(J_n)_{i,j}/(n+2)^{i-1}; i,j = 1, 2, ..., j', j'+1.$ Define J,* to be the matrix with the general element equal to

$$(J_n^*)_{i,j} = e_{i,j}$$

 $(J_n^*)_{ij} = e_{ij}$ In other words, J_n^* is the matrix obtained from J_n by extracting the factor 2 from each column and the factor $(n+2)^{i-1}$ from the i-th row.

Let n = 2s-1. By formula (1) of PART IB and the symmetry property $R_n^{(-p)}$ $= R_n^{(p-n)}$ one has

$$\begin{split} (\mathsf{J}_n)_{i,j} - (\mathsf{J}_n)_{i,j-1} &= 2[R_n^{(-j+1)}(i) - R_n^{(-j+2)}(i)] \\ &= 2\Big[-\sum_{t=0}^{j-2} (t+1)R_n^{(-t)}(i-1) + \sum_{t=j-1}^{n} (n-t+1)R_n^{(-t)}(i-1) \Big] \\ &= 2\sum_{t=j-1}^{n-j+1} (n-t+1)R_n^{(-t)}(i-1) = 2\sum_{t=j-1}^{s-1} (n+2)R_n^{(-t)}(i-1) \Big] \end{split}$$

Inserting of s = (n+1)/2 = j'+1 gives

$$(J_n)_{ij} - (J_n)_{i \ j-1} = 2(n+2) \sum_{t=j-1}^{j'} R_n^{(-t)}(i-1)$$
Therefore,
$$(J_n^*)_{ij} - (J_n^*)_{i \ j-1} = \sum_{t=j-1}^{j'+1} e_{i-1 \ t}; \qquad j \ge 2$$

$$(3.1)$$

Now we can derive the explicit formula for detd, * as follows.

$$\det J_{n}^{*} = \det \begin{bmatrix} 1 & 1 & \dots & 1 & 1 \\ e_{21} & e_{22} & \dots & e_{2} & j' & e_{2} & j'+1 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ e_{j'-1} & 1 & e_{j'-1} & 2 & \dots & e_{j'-1} & j' & e_{j'-1} & j'+1 \\ e_{j'} & 1 & e_{j'} & 2 & \dots & e_{j'} & j' & e_{j'} & j'+1 \\ e_{j'+1} & 1 & e_{j'+1} & 2 & \dots & e_{j'+1} & j' & e_{j'+1} & j'+1 \end{bmatrix}$$

$$= \det \begin{bmatrix} 1 & 0 & & \dots & 0 \\ e_{21} & j' & & \dots & 1 \\ \vdots & \vdots & & \vdots & \vdots & \vdots \\ e_{j'-1} & 1 & e_{j'-2} & 2^{+e} & j'-2 & 3^{+} & \dots^{+e} & j'-2 & j'+1 & \dots & e_{j'-2} & j'+1 \\ e_{j'} & 1 & e_{j'-1} & 2^{+e} & j'-1 & 3^{+} & \dots^{+e} & j'-1 & j'+1 & \dots & e_{j'-1} & j'+1 \\ e_{j'+1} & 1 & e_{j'} & 2^{+e} & j' & 3^{+} & \dots^{+e} & j' & j'+1 & \dots & e_{2} & j'+1 \\ \vdots & \vdots & & \vdots & & \vdots & & \vdots \\ e_{j'} & 2^{+e} & 2^{3} & \dots & e_{2} & j'+1 & \dots & e_{2} & j'+1 \\ \vdots & \vdots & & & \vdots & & \vdots \\ e_{j'} & 2^{+e} & j' & 3^{+} & \dots^{+e} & j' & j'+1 & e_{2} & j'+1 & \dots & e_{j'} & j'+1 \end{bmatrix}$$

$$= \det \begin{bmatrix} 1 & 1 & \dots & 1 \\ e_{22} & e_{23} & \dots & e_{2} & j'+1 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ e_{j'} & 2^{+e} & j' & 3^{+} & \dots^{+e} & j' & j'+1 & \dots & e_{j'} & j'+1 \end{bmatrix}$$

$$= \det \begin{bmatrix} 1 & 1 & \dots & 1 \\ e_{22} & e_{23} & \dots & e_{2} & j'+1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ e_{j'} & 2^{-e} & j' & 3 & \dots & e_{j'} & j'+1 \end{bmatrix}$$

Note that the above determinant is a subdeterminant obtained from $\det J_n^*$ by deleting the first column and the last row. Repeating the above process will lead to

$$= \det \begin{bmatrix} 1 & 1 & \dots & 1 \\ e_{22} & e_{23} & \dots & e_{2} & j'+1 \\ e_{32} & e_{33} & \dots & e_{3} & j'+1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ e_{j'} & 2 & e_{j'} & 3 & \dots & e_{j'} & j'+1 \end{bmatrix} = \det \begin{bmatrix} 1 & 1 & \dots & 1 \\ e_{23} & e_{24} & \dots & e_{2} & j'+1 \\ e_{33} & e_{34} & \dots & e_{3} & j'+1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ e_{j'-1} & 3 & e_{j'-1} & 4 & \dots & e_{j'-1} & j'+1 \end{bmatrix}$$

$$= \dots = \det \begin{bmatrix} 1 & 1 \\ e_{2} & j' & e_{2} & j'+1 \end{bmatrix} = \det [1] = 1$$

Consequently, by the relation between J_n and J_n^* we have $\det J_n = 2^{j'+1}(n+2)^{1+2+\cdots+j'}\det J_n^* = 2^{(n+1)/2}(n+2)^{(n-1)/8}$ An illustration for n=7 is given below. (3.2)

$$J_{7}^{*} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 4 & 7 & 9 & 10 \\ 30 & 56 & 75 & 85 \\ 246 & 462 & 622 & 707 \end{bmatrix}, det J_{7}^{*} = det \begin{bmatrix} 1 & 0 & 0 & 0 \\ 4 & 3 & 2 & 1 \\ 30 & 7+9+10 & 9+10 & 10 \\ 246 & 56+75+85 & 75+85 & 85 \end{bmatrix}$$
$$= det \begin{bmatrix} 3 & 2 & 1 \\ 7+9+10 & 9+10 & 10 \\ 56+75+85 & 75+85 & 85 \end{bmatrix} = det \begin{bmatrix} 1 & 1 & 1 \\ 7 & 9 & 10 \\ 56 & 75 & 85 \end{bmatrix} = det \begin{bmatrix} 1 & 1 \\ 9 & 10 \end{bmatrix} = 1$$

(b) n is even

Let n=2s. Then j'=s. Introduce $e_{ij}=(1/2)(J_n)_{ij}/[(n+2)/2]^{i-1}$ for $i=1,2,\ldots,j'+1;\ j=1,2,\ldots,j'$ and $e_{i\ j'+1}=(J_n)_{i\ j'+1}/[(n+2)/2]^{i-1}$ for $i=1,2,\ldots,j'+1$. Define J_n* to be the matrix satisfying $(J_n*)_{ij}=e_{ij}$. Denote by $J_n*(h)$ the submatrix of J_n* obtained by deleting the i-th columns for $i=1,2,\ldots,j'+1-h$ and the j-th rows for $j=h+1,h+2,\ldots,j'+1$. In a similar way as in Case (a) we have when $2\leq j\leq j'$

$$\begin{array}{c} (\mathsf{J}_n)_{ij} - (\mathsf{J}_n)_{i,j-1} &= 2[R_n^{(-j+1)}(i) - R_n^{(-j+2)}(i)] \\ &= 2\sum_{t=j-1}^{n-j+1} (n-t+1)R_n^{(-t)}(i-1) &= 2\Big[\sum_{t=j-1}^{g-1} (n+2)R_n^{(-t)}(i-1) - (n-g+1)R_n^{(-g)}(i-1)\Big] \\ &= (n+2)\Big[\sum_{t=j-1}^{j-1} 2R_n^{(-t)}(i-1) + R_n^{(-j')}(i-1)\Big] \end{array}$$

and when
$$j = j'$$
:

$$(J_n^*)_{i,j} - (J_n^*)_{i,j-1} = 2\sum_{t=j}^{j'} e_{i-1,t} + e_{i-1,j'+1}$$

In a similar way as in Case (a) we reach at
$$\det J_n^* = 2^{j^*-1} \det J_n^*(j^*) = 2^{j^*-1} 2^{j^*-2} \det J_n^*(j^*-1)$$

$$= 2^{j^*-1} 2^{j^*-2} 2^{j^*-3} \cdot \dots \cdot 2^2 2 \det J_n^*(1) = 2^{(n^2-2n)/8}$$

Consequently,

$$\det J_n = 2^{j'} [(n+2)/2]^{1+2+\cdots+j'} \det J_n^* = (n+2)^{(n^2+2n)/8}$$
(3.3)

In the following we give an illustration for n=6.

$$J_{6}^{*} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 7 & 12 & 15 & 16 \\ 84 & 154 & 200 & 216 \\ 1092 & 2016 & 2632 & 2848 \end{bmatrix}, \quad \det J_{6}^{*} = \det \begin{bmatrix} 1 & 0 & 0 & 0 \\ 7 & 2(1+1)+1 & 2+1 & 1 \\ 84 & 2(12+15)+16 & 2\times15+16 & 16 \\ 1092 & 2(154+200)+216 & 2\times200+216 & 216 \end{bmatrix}$$

$$= \det \begin{bmatrix} 2 & 2 \\ 1 & 1 & 1 \\ 12 & 15 & 16 \\ 154 & 200 & 216 \end{bmatrix} = 2^{2} \det \begin{bmatrix} 1 & 0 & 0 \\ 12 & 2 \times 1 + 1 & 1 \\ 154 & 2 \times 15 + 16 & 16 \end{bmatrix} = 2^{2} \det \begin{bmatrix} 1 & 1 \\ 15 & 16 \end{bmatrix} = 2^{2+1} = 2^{3}$$

Therefore, $\det J_{\zeta} = 2^3 4^6 \det J_{\zeta}^* = 2^6 4^6 = 8^6$.

4. THE PROOF OF CONJECTURE A OF PART III

By eqn. (2.5) we can rewrite Conjecture A as
$$u(j'+1, 1)R_{n}^{(-j')}(2) = -u(j', 1)$$
 (4.1)

We need to derive the formulas for u(j'+1, 1) and u(j', 1).

(a) n is odd

By the definition of
$$u(j'+1, 1)$$
 we have
$$u(j'+1, 1) = (-1)^{(j'+2)} 2^{j'} (n+2)^{1+2+\dots+(j'-1)} \det J_n^{**}$$

where J_n^{**} is the submatrix of J_n^* obtained by deleting the first column and the last row. We already know from Section 3 that detd ** = 1. Thus

$$u(j'+1,1) = (-1)^{j'} 2^{(n-1)/2} (n+2)^{(n^2-4n+3)/8}$$
(4.2)

Now we concentrate on u(j',1). Bearing in mind eqn. (3.1) we can derive this quantity as follows.

where $\Delta = 1 + 2 + \dots + (j'-2) + j' = (n^2 - 4n + 11)/8$. Inserting of

 $e_{2j'+1} = (1/2)(J_n)_{2j'+1}/(n+2) = R_n^{(-j')}(2)/(n+2)$ into the above equation yields $u(j',1) = (-1)^{j'+1} 2^{(n-1)/2} (n+2)^{(n^2-4n+3)/8} R_n^{(-j')}(2)$ (4.3)

An illustration is given for n=9 in the following.

$$u(4,1) = 2^{4}11^{7} det \begin{bmatrix} 1 & 1 & 1 & 1 \\ 9 & 12 & 14 & 15 \\ 105 & 146 & 175 & 190 \\ 15873 & 22187 & 26703 & 29056 \end{bmatrix} = 2^{4}11^{7} det \begin{bmatrix} 1 & 0 & 0 & 0 \\ 9 & 1 & 1 & 1 \\ 105 & 12 & 14 & 15 \\ 15873 & 1798 & 2163 & 2353 \end{bmatrix}$$

$$= 2^{4}11^{7} \det \begin{bmatrix} 1 & 0 & 0 \\ 12 & 1 & 1 \\ 1798 & 175 & 190 \end{bmatrix} = 2^{4}11^{7} \det \begin{bmatrix} 1 & 0 \\ 175 & 15 \end{bmatrix} = 2^{4}11^{6} (11 \times 15),$$

where $11 \times 15 = R_{q}^{(-4)}$.

Conjecture A is a direct consequence of egns. (4.2) and (4.3).

(b) n is even

An analogous reasoning as in the case when n is odd yields

$$u(j'+1, 1) = (n+2)^{(n^2-2n)/8}$$

 $u(j',1) = (n+2)^{(n^2-2n)/8} R_n^{(-j')} (2)$

which indicates that Conjecture A is valid for even n.

REFERENCES

¹Article series "(ON) THE NUMBER OF KEKULÉ STRUCTURES FOR RECTANGLE-SHAPED BENZENOIDS:

PART IA - S.J. Cyvin, B.N. Cyvin and J.L. Bergan, Match 19, 189 (1986).

IB - R.S. Chen, Match 21, 259 (1986).

IIA - S.J. Cyvin, Match 19, 213 (1986).

IIB - R.S. Chen, Match 21, 277 (1986).

III - R.S. Chen, S.J. Cyvin and B.N. Cyvin, Match 22, 111 (1987).

IV - S.J. Cyvin, R.S. Chen and B.N. Cyvin, Match 22, 129 (1987).

V - S.J. Cyvin, B.N. Cyvin, J. Brunvoll, R.S. Chen and L.X. Su, Match 22, 141 (1987).

VI - S.J. Cyvin, B.N. Cyvin and R.S. Chen, Match 22, 151 (1987).