match no. 21 pp. 285-289 1986

ENUMERATION OF KEKULÉ STRUCTURES: TRIANGLE-SHAPED BENZENOIDS

S. J. CYVIN

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

(Received: December 1986)

Abstract: The enumeration problem of Kekulé structures for the benzenoid class of prolate triangles has been solved previously. Here the considerations are extended to oblate and intermediate triangles.

This is a continuation of the work on the number of Kekulé structures of classes of mirror-symmetrical pericondensed benzenoids.

Definitions. When n=1 for the mirror-symmetrical pentagons treated in the previous articles,[1,2] viz. $D^{i}(m,n)$ and $D^{j}(m,n)$, they reduce to triangular-shaped benzenoids or triangles. Specifically we define (a) the prolate triangle as

$$T^{i}(m) = D^{i}(m,1)$$

and (b) the oblate triangle as

$$T^{j}(m) = D^{j}(m,1);$$

see Figure 1. Prolate and oblate benzenoids have, as usual[3,4] the indentation inwards and outwards, respectively. It is useful to define an additional class, say $T(m)$, the intermediate triangle; see Fig. 1(c). This type of benzenoids may be created by (a) deleting an end hexagon from a prolate triangle or (b) adding a hexagon at the end of an oblate triangle. Figure 1 illustrates these features.

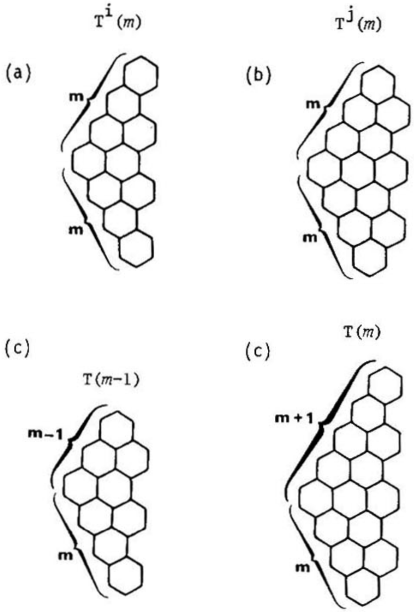

Fig. 1. The definitions of (a) prolate triangle, (b) oblate triangle and (c) intermediate triangle.

Connections between K numbers. The numbers of the Kekulé structures (K) for the three classes of triangles are inter-connected. An abbreviated notation is defined in the heading of Table 1. In terms of these symbols the following recurrence properties are valid.

$$T_m^{\,i} = T_{m-1}^{\,i} + T_{m-1} \; ; \qquad m \geq 1 \tag{1}$$

$$T_m = T_m^{\,j} + T_{m-1} \; ; \qquad m \geq 1 \tag{2}$$

As initial conditions one has

$$T_0^{\,i} = T_0^{\,j} = T_0 = 1 \tag{3}$$

Table 1. Numerical values of:

$$K\{\mathrm{T}^{\mathrm{i}}(m)\} = T_m^{\ \mathrm{i}}, \quad K\{\mathrm{T}^{\mathrm{j}}(m)\} = T_m^{\ \mathrm{j}}, \quad K\{\mathrm{T}(m)\} = T_m .$$

m	$T_m^{\ \mathrm{i}}$	$T_m^{\ \mathrm{j}}$	T_m
0	1	1	1
1	2	2	3
2	5	6	9
3	14	19	28
4	42	62	90
5	132	207	297
6	429	704	1 001
7	1 430	2 431	3 432
8	4 862	8 502	11 934
9	16 796	30 056	41 990
10	58 786	107 236	149 226

The information (1)-(3) is not sufficient to deduce successively the numbers for increasing m values. A necessary additional piece of information is reported in the subsequent paragraph.

Prolate triangle. During a previous work on truncated parallelograms[5] a triangular benzenoid was considered as an example. It is virtually identical with our prolate triangle. By means of an algorithm the following result was obtained for its K numbers.[5]

$$T_0^{\ \mathrm{i}} = \binom{0}{0} = 1 ,$$

$$T_1^{\ \mathrm{i}} = \binom{2}{1} = 2 ,$$

$$T_m^{\ \mathrm{i}} = \binom{2m}{m} - \sum_{i=0}^{m-2} T_i^{\ \mathrm{i}} \binom{2m-2-2i}{m-i} ; \qquad m \geq 2 \tag{4}$$

Now all the numbers $T_m^{\ \mathrm{i}}$ are accessible. From the recurrence relations (1) and (2) one obtains for the other types of triangles:

$$T_m{}^{\mathrm{j}} = T_{m+1}{}^{\mathrm{i}} - 2T_m{}^{\mathrm{i}} + T_{m-1}{}^{\mathrm{i}} \; ; \qquad m \geq 1 \tag{5}$$

$$T_m = T_{m+1}{}^{\mathrm{i}} - T_m{}^{\mathrm{i}} \tag{6}$$

Oblate triangle. For the sake of completeness we also report the relations of the type (4) for the oblate and intermediate triangles. In the former case one has

$$T_0{}^{\mathrm{j}} = \binom{0}{0} = 1 \; ,$$

$$T_1{}^{\mathrm{j}} = \binom{2}{1} = 2 \; ,$$

$$T_2{}^{\mathrm{j}} = \binom{4}{2} = 6 \; ,$$

$$T_m{}^{\mathrm{j}} = \binom{2m}{m} - \sum_{i=0}^{m-3} T_i \binom{2m-3-2i}{m-i} \; ; \qquad m \geq 3 \tag{7}$$

where

$$T_i = \sum_{k=0}^{i} T_k{}^{\mathrm{j}} \tag{8}$$

Intermediate triangle. Finally we have the following set of equations for the class of intermediate triangles.

$$T_0 = \binom{1}{0} = 1 \; ,$$

$$T_1 = \binom{3}{1} = 3 \; ,$$

$$T_m = \binom{2m+1}{m} - \sum_{i=0}^{m-2} T_i \binom{2m-2-2i}{m-i} \; ; \qquad m \geq 2 \tag{9}$$

Conclusion. A complete solution of the enumeration problem for Kekulé structures of the prolate, oblate and intermediate triangles is given. A preliminary set of recurrence relations, viz. eqns. (1) and (2), is an in-complete solution. The complete solutions, viz. eqns. (4), (7) and (9), are recurrence relations of a type not frequently encountered in the Kekulé structure enumerations. The number of terms accumulate with increasing *m*. More direct solutions have not been achieved.

Numerical *K* values up to *m*=10 are collected in Table 1.

REFERENCES

1 B.N. Cyvin, S.J. Cyvin and J. Brunvoll, Match

2 S.J. Cyvin and B.N. Cyvin, Match

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

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

5 S.J. Cyvin and I. Gutman, Match 19, 229 (1986).