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ENUMERATION OF KEKULÉ STRUCTURES: PENTAGON-SHAPED BENZENOIDS - PART I

B. N. CYVIN, S. J. CYVIN and J. BRUNVOLL

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

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Abstract: The enumeration problem for Kekulé structures is solved for a benzenoid class referred to as the 7-tier oblate pentagons. The fully computerized method is applied.

Among the pericondensed benzenoid classes[1] for which the Kekulé structures have been enumerated, the highly symmetrical ones (dihedral and mirror-symmetrical) have been studied by most authors.[2-8]

A regular t-tier strip[9,10] is defined as consisting of t rows of hexagons, where the number of hexagons in the top and bottom row is equal, say n. The left and right rims of the system are connected chains of t hexagons each. A certain class of t-tier strips can be dihedral or mirror-symmetrical for every value of n only when t is an odd number. The 5-tier strips have been studied systematically[9] and contain such highly symmetrical classes. For all the classes of 5-tier strips the combinatorial formulas for the number of Kekulé structures (K) as polynomials in n have been reported.[9] A general solution for K exists for hexagons[2,10] and chevrons.[2,11] The dihedral 7-tier hexagon has been treated in particular by Ohkami and Hosoya.[6] The multiple zigzag chains are mirror-symmetrical for an odd number of rows. A formula of K for 7 rows (a 7-tier strip) has been reported.[12] The general solution for a prolate rectangle[13] was first given by Yen.[3] The problem of oblate rectangles is considerably more difficult; the K formula for the 7-tier strip of this kind was deduced by Cyvin et al.,[13] and for the 9-tier oblate rectangle by Cyvin.[14]

In the present work the benzenoid classes of pentagons are treated.

The K formula is reported for the 7-tier oblate pentagon for the first time. The widely used method of fragmentation due to Randić[15] failed to be applicable in this case. As a whole the problem turned out to be rather difficult and therefore challenging. The only approach which met with success was the fully computerized method.[13,14]

Definition. Figure 1 shows the definition of mirror-symmetrical oblate pentagons, $D^j(m,n)$, where examples with m=3 (5-tier strip) and m=4 (7-tier strip) are depicted. One of the rims (chosen as the left) has the same shape as in the $O(m,n)$ hexagon, while the other (right) has an indentation outwards.

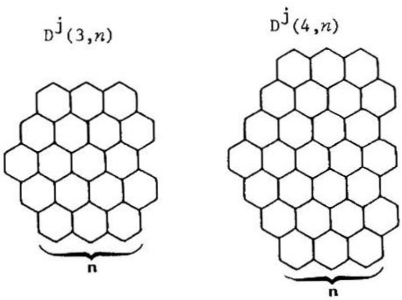

Fig. 1. Mirror-symmetrical oblate pentagons.

Derivation of the formula. For the number of Kekulé structures of the 5-tier mirror-symmetrical oblate pentagon it was found[9]

$$K\{D^j(3,n)\} = \frac{1}{4\cdot 6!}(n+1)(n+2)^2(n+3)^2(n+4)(3n^2 + 15n + 20) \quad (1)$$

In the following the corresponding formula is derived for $D^j(4,n)$.

Table 1 shows the numerical values for n up to 10 obtained from a computer program. For the sake of convenience we introduce the notation

$$D^j(n) = K\{D^j(4,n)\} \quad (2)$$

As the basis of the fully computerized method[13,14] it was assumed

Table 1. Numerical values of the number of Kekulé structures (K) for 7-tier oblate pentagons.

n	$K\{D^j(4,n)\}$	n	$K\{D^j(4,n)\}$
1	62	6	3 256 308
2	1 315	7	12 991 770
3	15 218	8	45 316 557
4	118 188	9	141 547 978
5	690 480	10	403 129 727

$$D^j(n) = (n+1)(n+2)^2(n+3)^2(n+4)P(n) \qquad (3)$$

where

$$P(n) = A + Bn + C\binom{n}{2} + D\binom{n}{3} + E\binom{n}{4} + F\binom{n}{5} + G\binom{n}{6} + H\binom{n}{7} \qquad (4)$$

The coefficients of (4) were determined by means of the K values of $n = 1, 2, \ldots, 7$ (Table 1) along with the trivial value $D^j(0) = 1$. It was found

$$A = \frac{1}{144}, \quad B = \frac{13}{360}, \quad C = \frac{149}{1440}, \quad D = \frac{1283}{7200}, \quad E = \frac{19}{100},$$

$$F = \frac{69}{560}, \quad G = \frac{5}{112}, \quad H = \frac{1}{144} \qquad (5)$$

A general validity of eqn. (4) with the coefficients (5) is not proved.

Firstly, the form (3) implies that $D^j(n)$ should be a polynomial in n of 13-th degree. We can at least say with confidence that the degree is less than 16. That is namely the degree pertaining to the hexagon $O(4,n)$. The removing of corners[10] leads to a lowering of the degree of the corresponding K formulas. Thus for instance $K\{O(3,n)\}$ is a polynomial of 9-th degree,[9] while $K\{D^j(3,n)\}$ has the degree 8. Here $D^j(3,n)$ is simply the hexagon $O(3,n)$ with one corner removed. In the present case the $D^j(4,n)$ benzenoid is obtained not only by removing one corner from the hexagon $O(4,n)$, but a further indentation is imposed.

Secondly, the linear factors of eqn. (3) were strictly speaking assumed as a working hypothesis only. They are highly probable, however, from the analogy on the basis of a great number of similar formulas.[9,10,13,14]

The chances that eqn. (4) is correct are highly increased by the fact that the three highest K numbers of Table 1, not used in the computation of the coefficients (5), were found to be reproduced exactly by the formula. In conclusion we suppose with almost certainty that we have derived the general formula. It was transferred to the factored polynomial form with the result

$$D^{j}(n) = K\{D^{j}(4,n)\}$$

$$= \frac{1}{10!}(n+1)(n+2)^{2}(n+3)^{3}(n+4)^{2}(n+5)(5n^{4} + 60n^{3} + 271n^{2} + 546n + 420) \quad (6)$$

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