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

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Abstract: A combinatorial formula for the number of Kekulé structures for the benzenoid class of 7-tier prolate pentagons is developed. The solution is obtained by a direct analysis involving an auxiliary benzenoid class. A formula for the 9-tier prolate pentagons is tentatively forwarded by extrapolation.

In the systematic studies of the number of Kekulé structures (K) of highly symmetrical (dihedral or mirror-symmetrical) pericondensed benzenoids (cf. Ref. 1 and references cited therein) it is natural to attack the problem of mirror-symmetrical prolate pentagons; cf. Fig. 1.

For the 5-tier mirror-symmetrical prolate pentagon it was found[2]

$$K\{D^{i}(3,n)\} = \frac{1}{180}(n+1)(n+2)^{2}(n+3)(2n+3)(2n+5) \tag{1}$$

In this paper we deduce the combinatorial formula of K for $D^{i}(4,n)$. In contrast to the case of the oblate pentagon,[1] $D^{j}(4,n)$, it was found possible to use the same methods of a direct analysis as in the case of the oblate rectangle.[3]

Seven-tier prolate pentagon without apex. Figure 2 defines a benzenoid class of 7-tier prolate pentagons without apex, $Da^{i}(4,n)$. If the enumeration problem is solved for this class we have for the pentagon in question:

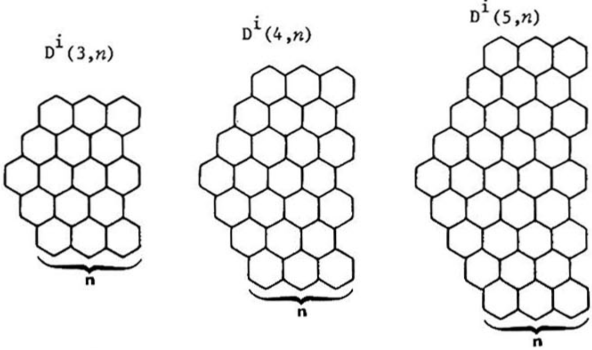

Fig. 1. Mirror-symmetrical prolate pentagons.

$$K\{D^{i}(4,n)\} = \sum_{i=0}^{n} K\{Da^{i}(4,i)\} \tag{1}$$

In Ref. 3 the auxiliary class $B(n,\ 3,\ -l)$ is defined. The methods used in that work lead to

$$K\{Da^{i}(4,n)\} = \sum_{i=0}^{n} [K\{B(n,\ 3,\ -i)\}]^{2} \tag{2}$$

A systematic study of the auxiliary classes of the type needed here has

Fig. 2. The 7-tier prolate pentagon without apex.

given the so far unpublished result:

$$K\{B(n,\ 3,\ -l)\} = (n-l+1)\binom{n+3}{3} - (n+2)\binom{n-l+2}{3} \tag{3}$$

On inserting into eqn. (2) one obtains

$$K\{Da^{i}(4,n)\} = \binom{n+3}{3}^2 \sum_{j=0}^{n} (j+1)^2$$

$$- 2(n+2)\binom{n+3}{3} \sum_{j=0}^{n} (j+1)\binom{j+2}{3} + (n+2)^2 \sum_{j=1}^{n} \binom{j+2}{3}^2 \tag{4}$$

All the summations in (4) are conveniently expressed in terms of the K number formulas for chevrons:[4]

$$\sum_{j=0}^{n} (j+1)^2 = K\{Ch(2,2,n)\}\ ,$$

$$\sum_{j=0}^{n} (j+1)\binom{j+2}{3} = K\{Ch(2,4,n)\} - K\{Ch(2,3,n)\}\ ,$$

$$\sum_{j=1}^{n} \binom{j+2}{3}^2 = K\{Ch(4,4,n)\} - \binom{n+3}{3}^2 \tag{5}$$

The chevron formulas were expressed in terms of polynomials in n and inserted into (4). The answer was reduced to

$$K\{Da^{i}(4,n)\} = \frac{1}{7560}(n+1)(n+2)^2(n+3)(2n+3)(2n+5)(4n^2+16n+21) \tag{6}$$

Seven-tier prolate pentagon. The expression from (6) was inserted into (1) and gave by an elementary, but tedious analysis:

$$K\{D^{i}(4,n)\} = \frac{1}{7560}\left[16 \sum_{i=0}^{n} (i+1)^9 + 144 \sum_{i=0}^{n} (i+1)^8\right.$$

$$+ 576 \sum_{i=0}^{n} (i+1)^7 + 1344 \sum_{i=0}^{n} (i+1)^6 + 1995 \sum_{i=0}^{n} (i+1)^5$$

$$+ 1911 \sum_{i=0}^{n} (i+1)^4 + 1139 \sum_{i=0}^{n} (i+1)^3 + 381 \sum_{i=0}^{n} (i+1)^2$$

$$\left. + 54 \sum_{i=0}^{n} (i+1) \right] \quad (7)$$

The summations of (7) were worked out, and the expression was simplified to the final result:

$$K\{\mathrm{D}^{\mathrm{i}}(4,n)\} = \frac{1}{75600}(n+1)(n+2)^2(n+3)^2(n+4)(2n+3)(2n+5)^2(2n+7) \quad (8)$$

Table 1 shows numerical values.

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

n	$K\{\mathrm{D}^{\mathrm{i}}(4,n)\}$	n	$K\{\mathrm{D}^{\mathrm{i}}(4,n)\}$
1	42	6	395 352
2	594	7	1 215 126
3	4 719	8	3 331 251
4	26 026	9	8 321 170
5	111 384	10	19 240 650

Nine-tier prolate pentagon. A 9-tier prolate pentagon is depicted in Fig. 1 (right).

The formulas of $K\{\mathrm{D}^{\mathrm{i}}(m,n)\}$ were found to consist of linear factors in n only; see eqn. (8) for m=4 and (1) for m=3. For m=2 one has $\mathrm{D}^{\mathrm{i}}(2,n)$ = Ch(2,2,n), and finally (m=1) $\mathrm{D}^{\mathrm{i}}(1,n)$ = L(n). The formulas are well known, viz.[5]

$$K\{D^{i}(2,n)\} = \frac{1}{6}(n+1)(n+2)(2n+3) \tag{9}$$

$$K\{D^{i}(1,n)\} = n+1 \tag{10}$$

It is tempting to guess that all K formulas for $D^{i}(m,n)$ follow the same pattern. Specifically we set up the quotients for m+1 and m, viz.:

$$K\{D^{i}(2,n)\}/K\{D^{i}(1,n)\} = \frac{1}{6}(n+2)(2n+3) \tag{11}$$

$$K\{D^{i}(3,n)\}/K\{D^{i}(2,n)\} = \frac{1}{30}(n+2)(n+3)(2n+5) \tag{12}$$

$$K\{D^{i}(4,n)\}/K\{D^{i}(3,n)\} = \frac{1}{420}(n+3)(n+4)(2n+5)(2n+7) \tag{13}$$

By extrapolation we set up tentatively:

$$K\{D^{i}(5,n)\}/K\{D^{i}(4,n)\} = \frac{1}{3780}(n+3)(n+4)(n+5)(2n+7)(2n+9) \tag{14}$$

The constant factor causes no problems because

$$K\{D^{i}(m,0)\} = 1 \tag{15}$$

for every m. Thus in (14) the denominator is $3\cdot4\cdot5\cdot7\cdot9$. The net result from eqns. (8) and (14) is

$$K\{D^{i}(5,n)\} = \frac{1}{285768000}(n+1)(n+2)^{2}(n+3)^{3}(n+4)^{2}(n+5)$$
$$\times(2n+3)(2n+5)^{2}(2n+7)^{2}(2n+9) \tag{16}$$

where the denominator is equal to $4^{3}\cdot5^{3}\cdot7^{2}\cdot9^{3}$.

It is very probable that the formula (16) is correct, although not rigorously proved. For n = 1, 2, 3, 4, 5, 6, 7 and 8 it was verified to give the correct (computer-checked) results, viz. 132, 4 719, 81 796, 884 884, 6 852 768, 41 314 284, 204 951 252 and 869 562 265, respectively.

Conclusion. The methods applied in the derivation of the formula of $K\{D^i(4,n)\}$ are well established, but turned out to be tedious. The $K\{D^i(5,n)\}$ formula resulted from guess-work. The forms of the formulas for $D^i(m,n)$ suggest that it should be possible to derive them in a simpler way, arriving directly at the linear factors. So far no such procedure has been detected.

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