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Di-4-Catafusenes: A New Class of Polygonal Systems Representing Polycyclic Conjugated Hydrocarbons*

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Di-4-catafusenes are defined as catacondensed polygonal systems consisting of two tetragons each and otherwise only hexagons. Di-4-catafusenes are enumerated by combinatorial constructions and by computer programming. For the unbranched systems (nonhelicenic + helicenic), as the main result of the present work, a complete mathematical solution is reported. A new algebraic approach has been employed, which involves a triangular matrix with some interesting mathematical properties.

INTRODUCTION

Polygonal systems[2,3] are chemical graphs[4] which represent condensed polycyclic conjugated hydrocarbons. In precise terms, a polygonal system is a system consisting of simply connected polygons, where any two polygons either share exactly one edge or are disjoint. Many subclasses of polygonal systems have been defined. For instance, biphenylenoids[5] consist of exactly one tetragon each and otherwise only hexagons. A similar subclass of polygonal systems is introduced in the present work. Only catacondensed systems, *viz.* those without internal vertices, are considered here.

Definition: A di-4-catafusene is a catacondensed polygonal system consisting of exactly two tetragons and otherwise only hexagons (if any).

A prototype of di-4-catafusenes is $C_{18}H_{10}$ [3]phenylene or terphenylene, which has been synthesized both in the angular[6,7] and in the linear form.[8–11]

* Dedicated to Professor Nenad 13-ić[1], on the occasion of his appointment to the position of Editor-in-Chief of this Journal.

Many theoretical investigations have been conducted on different polygonal systems with di-4-catafusenes among them.[2,12–30] These works deal with conjugated circuits, Kekulé and algebraic structure counts, local aromaticity, total π-electron energy, cyclic conjugation, *etc.* Some of them are devoted to [*h*]phenylenes, but none of them treat exclusively the systems defined here as di-4-catafusenes.

In the present work, the di-4-catafusenes were generated, enumerated and classified. Different methods were employed: combinatorial constructions, computer programming, and algebraic deductions. In particular, a complete mathematical solution was achieved for the unbranched systems by means of a new approach, which led to a special triangular matrix. The useful formulation in terms of generating functions[3,31] is applied to some extent.

The number of polygons (or rings) in a di-4-catafusene is identified by the symbol r. Then, the chemical formula reads $C_{4r-2}H_{2r}$.

COMBINATORIAL CONSTRUCTIONS

The smallest di-4-catafusenes (see Figure 1) were constructed by systematic drawings. Hereby the different positions of the two tetragons in relation to each other were considered. One might speak about »stratum« in analogy with the generation of double coronoids.[32]

COMPUTER PROGRAMMING

The method of combinatorial constructions described above is not particularly convenient for computerization. Instead, a computer algorithm was based on the generation of catacondensed benzenoids or catabenzenoids (consisting of hexagons only), followed by a conversion of two hexagons in each system to tetragons. A more detailed description of the procedure follows.

In a catabenzenoid, mark the L_1 and L_2 mode hexagons,[33,34] *viz.* the terminal and linearly annelated ones. Convert two of these hexagons to tetragons in all possible ways, assuring that isomorphic systems are avoided if the catabenzenoid has a symmetry higher than C_s, *viz.* D_{2h}, C_{2h}, or C_{2v}. Hereby the A_2 mode (angularly annelated) hexagons are neglected, since a conversion to tetragon will straighten out the system so that it becomes isomorphic with one already generated from conversion of L_2. Finally, an A_3 mode (branching) hexagon cannot be converted to a tetragon at all.

The described algorithm is illustrated in Figure 2. Symmetrically nonequivalent L_1 and L_2 mode hexagons are indicated by asterisks, the rest of them by dots. The numerals indicate how many nonisomorphic di-4-catafusenes are generated from each of the catabenzenoids.

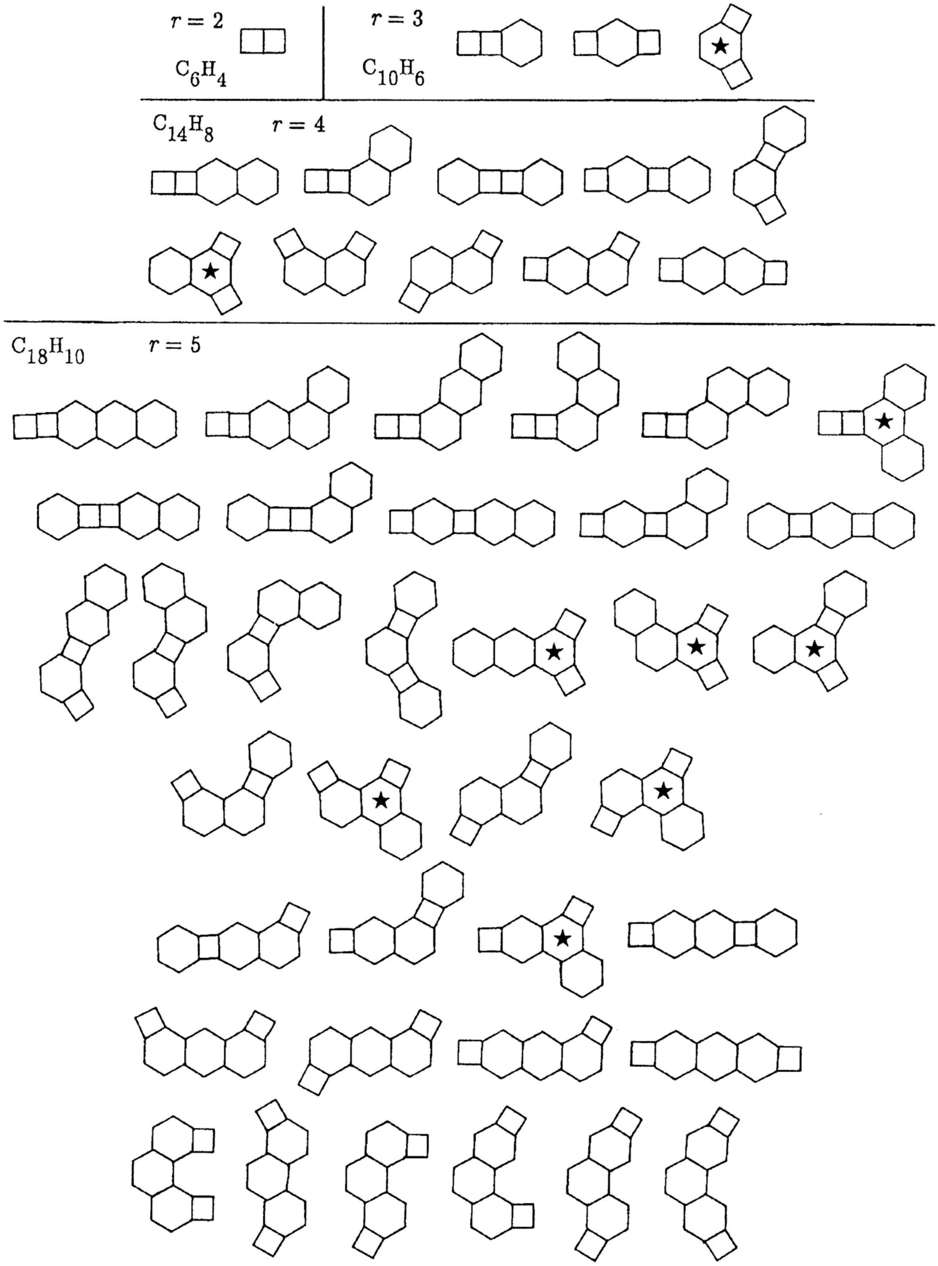


Figure 1. The 1, 3, 10 and 36 di-4-catafusenes with r = 2, 3, 4 and 5, respectively. Branching hexagons are marked with asterisks.

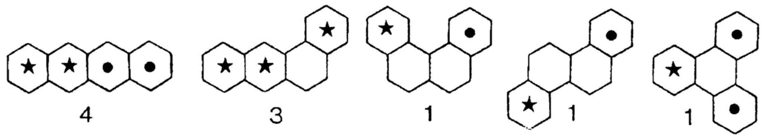


Figure 2. Generation of the 10 di-4-catafusenes with r = 4 by conversion of hexagons to tetragons in catabenzenoids.

TABLE I

Numbers of nonhelicenic unbranched di-4-catafusenes

r	D_{2h}	C_{2h}	C_{2v}	C_s	Total
2	1	0	0	0	1
3	1	0	2	0	3
4	2	1	3	3	9
5	2	1	9	17	29
6	3	6	11	78	98
7	3	6	29	308	346
8	4	25	33	1148	1210
9	4	25	86	4105	4220
10	5	91	90	14290	14476
11	5	91	260	48759	49115
12	6	314	262	163791	164373
13	6	312	796	543181	544295
14	7	1043	776	1781948	1783774
15	7	1035	2464	5791224	5794730

TABLE II

Numbers of nonhelicenic branched di-4-catafusenes

r	D_{2h}	C_{2h}	C_{2v}	C_s	Total
4	0	0	1	0	1
5	0	0	2	5	7
6	0	1	10	42	53
7	0	1	18	297	316
8	1	10	54	1736	1801
9	1	10	99	9391	9501
10	2	71	252	47819	48144
11	2	74	472	234663	235211
12	6	414	1078	1119630	1121128
13	6	435	2120	5236497	5239058
14	10	2188	4547	24118027	24124772
15	10	2310	9320	109798460	109810100

The numerical results are collected in Tables I and II for the unbranched and branched di-4-catafusenes, respectively. It is emphasized that the numbers pertain to geometrically planar or nonhelicenic[35] systems only. Nonhelicenic di-4-catafusenes are systems that can be generated from nonhelicenic catabenzenoids. On the other hand, helicenic di-4-catafusenes can be generated in the same way (by conversion of hexagons to tetragons) from catacondensed helicenes (helicenic catafusenes).[35]

ALGEBRAIC SOLUTION FOR UNBRANCHED SYSTEMS

Outline of the Method

A complete mathematical solution was deduced for the numbers of unbranched di-4-catafusenes, nonhelicenic and helicenic systems taken together. Basically, the same principles were used as on the classical enumeration of unbranched catafusenes by Balaban and Harary,[36] which has been revisited elsewhere.[35,37] The method[38] has been described under the name »stupid sheep counting« (where »stupid« refers to the counting not to the sheep).[3,39] The term »crude total« belongs to this description. The main line of the stupid sheep counting applied to the unbranched di-4-catafusenes is specified in the following.

For a given number of polygons (r), the crude total, J_r, counts the D_{2h} systems once, the C_{2h} and C_{2v} systems twice, and the C_s systems four times. Hence,

$$J_r = D_r + 2C_r + 2M_r + 4A_r \tag{1}$$

where D_r, C_r, M_r and A_r pertain to the symmetry groups in the same order as specified above. The total number of systems, say I_r, is simply

$$I_r = D_r + C_r + M_r + A_r \,. \tag{2}$$

On eliminating A_r from Eqs. (1) and (2), the following is obtained:

$$I_r = \frac{1}{4}(J_r + 3D_r + 2C_r + 2M_r) \,. \tag{3}$$

Hence, in order to solve the problem, one has to enumerate specifically the symmetrical (D_{2h}, C_{2h} and C_{2v}) systems, in addition to finding the crude totals.

The generating functions for the numbers of Eq. (3) are defined by:

$$I(x) = \sum_{r=2}^{\infty} I_r x^r\ ,\ J(x) = \sum_{r=2}^{\infty} J_r x^r\ ,\ D(x) = \sum_{r=2}^{\infty} D_r x^r\ ,$$

$$C(x) = \sum_{r=4}^{\infty} C_r x^r\ ,\ M(x) = \sum_{r=3}^{\infty} M_r x^r\ . \tag{4}$$

Triangular Matrices

Define the numbers:

$$a_{11} = 1, \qquad a_{(i+1)j} = 2a_{ij} + a_{i(j-1)} \tag{5}$$

while $a_{i0} = 0$, $a_{ij} = 0$ when $j > i$. Collect these numbers into a triangular ***A*** matrix as:

i/*j*	1	2	3	4	5	6
1	1					
2	2	1				
3	4	4	1			
4	8	12	6	1		
5	16	32	24	8	1	
6	32	80	80	40	10	1
....						

Additional sets of numbers are defined similarly by:

$$b_{11} = 1,\ b_{(i+1)j} = 2b_{ij} + b_{i(j-1)} + \delta_{(i+1)j} \tag{6}$$

while $b_{i0} = 0$, $b_{ij} = 0$ when $j > i$. Here, δ_{uv} is the Kronecker delta: $\delta_{uv} = 0$ when $u \neq v$, $\delta_{uu} = 1$. Another triangular matrix ***B*** is constructed:

i/*j*	1	2	3	4	5	6
1	1					
2	2	2				
3	4	6	3			
4	8	16	12	4		
5	16	40	40	20	5	
6	32	96	120	80	30	6
....						

The $\boldsymbol{A}$ and $\boldsymbol{B}$ matrices are closely related; it was proved that:

$$b_{ij} = \frac{1}{2} a_{(i+1)j} \ . \tag{7}$$

Crude Total

Elements of the $\boldsymbol{A}$ matrix are chosen so that the sum along a row gives the crude total for unbranched catafusenes[35] with $i + 1$ hexagons;

$$\sum_{j=1}^{i} a_{ij} = 3^{i-1} \ . \tag{8}$$

In matrix notation:

$$\boldsymbol{A} \ \{1, 1, 1, 1,...\} = \{1, 3, 9, 27,...\} \ . \tag{9}$$

Furthermore, the individual a_{ij} elements count the systems where $r = i + 1$ and $j + 1$ is the number of the L_1 and L_2 mode hexagons taken together. Therefore,

$$J_{i+1} = \sum_{j=1}^{i} \binom{j+1}{2} a_{ij} \ . \tag{10}$$

holds for the crude totals of unbranched di-4-catafusenes; in matrix notation:

$$\boldsymbol{A}\left\{\binom{2}{2}, \binom{3}{2}, \binom{4}{2}, \binom{5}{2}, \ldots\right\} = \{1, 5, 22, 90, \ldots\} \ . \tag{11}$$

The pertinent generating function in expanded form is

$$J(x) = x^2 + 5x^3 + 22x^4 + 90x^5 + 351x^6 + 1323x^7 + \ldots \tag{12}$$

where any number of the coefficients is accessible from the above relations.

Dihedral and Linear Mirror-Symmetrical Systems

The dihedral (D_{2h}) systems under consideration are linear, and their numbers are

$$D_r = \lfloor r/2 \rfloor \tag{13}$$

when $\lfloor X \rfloor$ (the floor of X) is the largest integer not larger than X. The corresponding generating function is:[3]

$$D(x) = x^2(1 - x)^{-1}(1 - x^2)^{-1} = x^2 + x^3 + 2x^4 + 2x^5 + 3x^6 + 3x^7 + \ldots \quad (14)$$

Let L_r be the number of linear mirror-symmetrical systems; they form a subclass of the M_r systems, which belong to C_{2v}. Then, by a little bit of combinatorics, where the stupid sheep counting can be evoked again, the following is found:

$$L_r = \frac{1}{2}\left\{\binom{r}{2} - \lfloor r/2 \rfloor\right\} \quad (15)$$

and the associated generating function

$$L(x) = x^3(1-x)^{-2}(1-x^2)^{-1} = x^3 + 2x^4 + 4x^5 + 6x^6 + 9x^7 + 12x^8 + \ldots. \quad (16)$$

Centrosymmetrical Systems

In the enumeration of the C_r centrosymmetrical (C_{2h}) systems, the $\boldsymbol{B}$ matrix comes into operation. The sum along a row of $\boldsymbol{B}$ gives the numbers of unbranched C_{2h} catafusenes[35] with $2i + 2$ and with $2i + 3$ hexagons:

$$\sum_{j=1}^{i} b_{ij} = \frac{1}{2}(3^i - 1)\ . \quad (17)$$

In matrix notation:

$$\boldsymbol{B}\ \{1, 1, 1, 1, \ldots\} = \{1, 4, 13, 40, \ldots\}\ . \quad (18)$$

Now, it is found for the di-4-catafusenes under consideration that

$$C_{2i+2} = C_{2i+3} = \sum_{j=1}^{i} j b_{ij} = \frac{1}{2}\sum_{j=1}^{i} j a_{(i+1)j}\ . \quad (19)$$

In matrix notation:

$$\boldsymbol{B}\ \{1, 2, 3, 4, \ldots\} = \{1, 6, 25, 92, \ldots\} \quad (20)$$

or

$$\frac{1}{2}(\boldsymbol{A} - \boldsymbol{I})\{1, 2, 3, 4, 5, ...\} = \{0, 1, 6, 25, 92, ...\} \tag{21}$$

where $\boldsymbol{I}$ is the identity matrix.

With regard to the formalism of generating functions, it is expedient to introduce c_i as expression (19), and

$$c(x) = \sum_{i=1}^{\infty} c_i x^i = x + 6x^2 + 25x^3 + 92x^4 + 321x^5 + 1090x^6 + \ldots \tag{22}$$

In terms of this function, one finds that

$$C(x) = x^2(1 + x)c(x^2) = x^4 + x^5 + 6x^6 + 6x^7 + 25x^8 + 25x^9 + ... \tag{23}$$

Mirror-Symmetrical Systems

The mirror-symmetrical (C_{2v}) unbranched di-4-catafusenes with numbers M_k are divided into three subclasses according to

$$M_k = L_k + C_k + K_k \ . \tag{24}$$

The numbers L_k pertain to the linear systems, which are treated above. The C_k systems stand in a one-to-one correspondence to the centrosymmetrical systems as *cis*/*trans* isomers.

There remains a class of K_k systems, which comes up for odd r values only. In a similar way as in the case of C_r, the following was found:

$$K_{2i+1} = \sum_{j=1}^{i} ja_{ij} \tag{25}$$

$$\boldsymbol{A}\{1, 2, 3, 4, ...\} = \{1, 4, 15, 54, ...\} \ . \tag{26}$$

In the formalism of generating functions, introduce k_i as expression (25).

Consequently,

$$k(x) = \sum_{i=1}^{\infty} k_i x^i = x + 4x^2 + 15x^3 + 54x^4 + \ldots \tag{27}$$

and

$$K(x) = \sum_{r=3}^{\infty} K_r x^r = xk(x^2) = x^3 + 4x^5 + 15x^7 + 54x^9 + 189x^{11} + \ldots \qquad (28)$$

Further Developments

The expressions in Eqs. (19) and (25) were obtained in explicit forms by a lengthy derivation, which will not be included here; the result is:

$$C_{2i+2} = C_{2i+3} = \frac{1}{2}\left[(i+3)\, 3^{i-1} - (i+1)\right] \qquad (29)$$

$$K_{2i+1} = (i+2)\, 3^{i-2}\ . \qquad (30)$$

In consequence, functions $c(x)$ and $k(x)$ of Eqs. (22) and (27), respectively, are obtainable in explicit forms. The following results were deduced:

$$c(x) = x(1 - 2x - x^2)(1 - x)^{-2}(1 - 3x)^{-2} \qquad (31)$$

$$k(x) = x(1 - 2x)(1 - 3x)^{-2}\ . \qquad (32)$$

Also, the crude total Eq. (10) was deduced in explicit form by tedious combinatorial considerations. Here, we only give the result:

$$J_{i+1} = \frac{1}{2}(i + 1)(i + 8)\, 3^{i-3}\ . \qquad (33)$$

The corresponding generating function (12) is

$$J(x) = x^2\,(1 - 4x + 4x^2)(1 - 3x)^{-3}\ . \qquad (34)$$

Complete Solution

The above analysis made it possible to express the I_r numbers of unbranched di-4-catafusenes by finite summation in terms of the a_{ij} elements, which are accessible through Eq. (5). The result is:

$$I_r = \frac{1}{4}\left[\sum_{j=1}^{r-1}\binom{j+1}{2}a_{(r-1)j} + \binom{r}{2}\right] + \frac{1}{2}\left[\sum_{j=1}^{\lfloor r/2\rfloor} ja_{\lfloor r/2\rfloor j} + \sum_{j=1}^{(r-1)/2} ja_{(r-1)/2(j)}\right]. \qquad (35)$$

It is understood that a_{tj} is equal to zero if t is not an integer; therefore, the last summation in Eq. (29) is effective only for r = 3, 5, 7,... . The sum-

TABLE III

Numbers of unbranched di-4-catafusenes (nonhelicenic + helicenic)

r	D_{2h}	C_{2h}	C_{2v}	C_s	Total
2	1	0	0	0	1
3	1	0	2	0	3
4	2	1	3	3	9
5	2	1	9	17	29
6	3	6	12	78	99
7	3	6	30	312	351
8	4	25	37	1183	1249
9	4	25	95	4313	4437
10	5	92	112	15388	15597
11	5	92	306	53928	54331
12	6	321	351	186651	187329
13	6	321	1005	639033	640365
14	7	1090	1132	2168938	2171167
15	7	1090	3326	7305104	7309527

mations can be substituted by virtue of relations (29), (30), and (33), yielding the following result:

$$I_r = \frac{1}{4}\left\{\frac{1}{2}r(r+7)3^{r-4} + \binom{r}{2} + 2\left[\lfloor r/2 \rfloor + 2\right]3^{\lfloor r/2 \rfloor - 2} + \frac{1}{2}\left[1-(-1)^r\right](r+3)3^{(r-5)/2}\right\}. \quad (36)$$

This formula is explicit in r. Finally, we give the corresponding generation function:

$$I(x) = \frac{1}{4}x^2[(1-4x+4x^2)(1-3x)^{-3} + (3-x)(1-x)^{-2}(1-x^2)^{-1} +$$
$$+ 4x^2(1-2x^2-x^4)(1-x)^{-1}(1-x^2)^{-1}(1-3x^2)^{-2} + 2x(1-2x^2)(1-3x^2)^{-2}] \,. \quad (37)$$

Numerical values of I_r, including the distributions of these numbers into different symmetry groups, are collected in Table III.

BACK TO COMBINATORIAL CONSTRUCTIONS

The totals in Tables I – III display the rapidly increasing series of integers when r increases. Very soon, these numbers seem to exceed all imaginable needs in organic chemistry. Nevertheless, the integer series of this

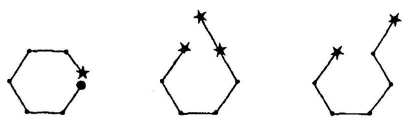
TABLE IV

Numbers of helicenic unbranched di-4-catafusenes

r	C_{2h}	C_{2v}	C_s	Total
6	0	1	0	1
7	0	1	4	5
8	0	4	35	39
9	0	9	208	217
10	1	22	1098	1121
11	1	46	5169	5216
12	7	89	22860	22956
13	9	209	95852	96070
14	47	356	386990	387393
15	55	862	1513880	1514797

kind have considerable interest in mathematical chemistry and in pure mathematics.[40] In order to be really useful, it is important that the deduced numbers are exact, no matter how large. This feature is important for several reasons. Firstly, subclasses of different systems are often enumerated in one way and may include small numbers even of chemical interest, but they may add up to large totals enumerated in a different way. Then, a check of the first calculations would be meaningless if one could not trust the large numbers to be exact. Secondly, enumerations may involve relatively small differences between large numbers. Examples of this case are treated in the following.

It is observed that the computer-generated numbers in Table I and the numbers from algebraic solutions in Table III are identical up to $r = 5$. This is as it should be and already a good check, since the smallest helicenic catafusene[35,36] is known to occur at $r = 6$. In general, the numbers of the helicenic systems under consideration are obtained by subtracting the numbers of Table I from those of Table III. The results are entered in Table IV. Here, for instance, the totals 39 and 217 (r = 8, 9) emerge from the differences 1249 − 1210 and 4437 − 4220, respectively.



1 3 1

Figure 3. Generation of the 5 helicenic unbranched di-4-catafusenes with r = 7 by conversion of hexagons to tetragons in catafusenes.

The method of combinatorial constructions (see above) was used to generate all the helicenic unbranched di-4-catafusenes for $r \leq 9$. This was a relatively easy task since the forms of the corresponding catafusenes are available.[35] As a pleasing fact, the relevant numbers of Table IV were indeed reproduced. The procedure is exemplified for $r = 7$ in Figure 3. It should be compared with Figure 2 with regard to the marking of hexagons and indicated numbers. However, representation in terms of dualists[4,35,36,41] is employed in Figure 3.

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SAŽETAK

Di-4-catafuzeni: nova klasa poligonskih sustava koji predstavljaju policikličke konjugirane ugljikovodike

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Di-4-katafuzeni definirani su kao katakondenzirani poligonski sustavi koji se sastoje od šesterokuta i točno dva četverokuta. Di-4-katafuzeni prebrojani su kombinatornim i računalnim postupcima. Kao glavni rezultat u radu, prikazano je cjelovito matematičko rješenje za nerazgranate sustave (helicinske i nehelicinske, zajedno). Pri tome je upotrijebljen nov algebarski pristup koji uključuje trokutastu matricu zaminljivih matematilčkih svojstava.