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Original Scientific Paper

Generation of Graphs of Unbranched Pentahexagonal Catacondensed Systems

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Enumeration of graphs of polycyclic unbranched pentahexagonal catacondensed systems is considered. A graph of this class is a ribbon of pentagonal and hexagonal rings connected with each other. The numbers of graphs with r rings for $3 \leq r \leq 13$ are presented.

INTRODUCTION

One of the rapidly developing trends in mathematical chemistry is a constructive enumeration of graphs of polycyclic systems including molecular graphs of polycyclic compounds. The problems arising here are similar to the problem of counting polyominoes of different types and they have various chemical and physical applications.[1–6] In organic chemistry, particular importance is attached to generating graphs of hexagonal systems modelling a structure of benzenoid hydrocarbons.[7–30] A number of papers are devoted to the enumeration of graphs consisting of triangular, tetragonal or pentagonal rings.[31–35] Chemical properties of polycyclic molecules depicted by graphs consisting of pentagonal and hexagonal rings have been studied by Randić *et al.*[37] The present contribution deals with the enumeration of graphs of unbranched pentahexagonal catacondensed systems.

GRAPHS OF PENTAHEXAGONAL SYSTEMS

A pentahexagonal system is a planar system of simply connected hexagons and pentagons. If all pentagons and hexagons are regular, then this definition includes nonplanar systems, which would possess overlapping edges if drawn in a plane. We consider graphs corresponding to unbranched catacondensed pentahexagonal systems. A graph of this class consists of pentagonal and hexagonal rings. Two arbitrary rings of a graph have either one common edge, *i.e.* they are adjacent, or have no common vertices. In catacondensed systems no three rings which share a common vertex. By placing each ring in correspondence with a new vertex and then joining them if the corresponding rings are adjacent, we get the characteristic graph of the initial one. A class of graphs of pentahexagonal systems consisting of r rings, for which their characteristic graph is isomorphic to a simple path, is denoted by PH_r. Vertices of the characteristic graph of degree 1 correspond to the terminal rings of a PH_r graph. All vertices of PH_r graphs have degree 2 or 3. Such a graph model certains classes of chemical compounds.[37] Among graphs shown in Figure 1, graphs G_1 and G_2 belong to the class PH_r.

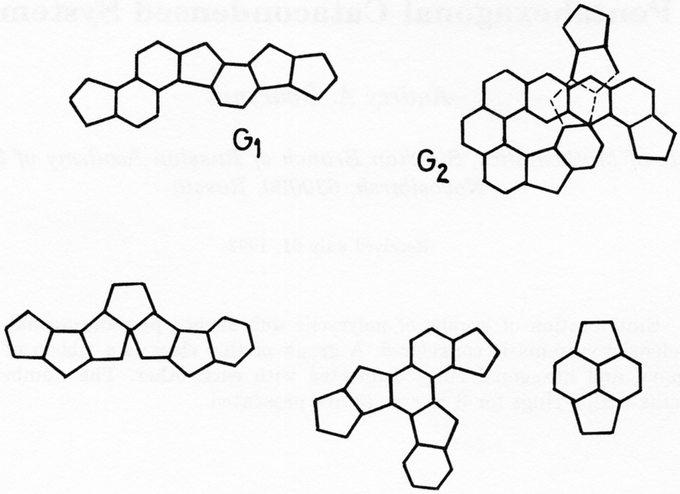

Figure 1. Graphs of pentahexagonal systems.

CLASSES OF PENTAHEXAGONAL SYSTEMS GRAPHS

A set of graphs of pentahexagonal systems can be represented as disjoint classes $PH_r = \bigcup_{p=0}^{r} S_p$ where class S_p includes graphs with p pentagonal and $h = r - p$ hexagonal rings. Classes of graphs composed solely of pentagonal and hexagonal rings are denoted by P_r and H_r, respectively. The number of vertices in a graph G of the class S_p is equal to $n(G) = 4h+3p+2$, and the number of edges is $m(G) = 5h+4p+1$.

Let x be the vector of ring sizes when graph rings are passed in a sequential manner, for instance $x = (5,6,6,5,6,5,5)$ for graph G_1 in Figure 1. Then each class S_p may be represented as $S_p = \bigcup_{x \in X} G_x$, where G_x is a set of graphs generated by vector x of ring sizes from set X of all such different vectors.

ALGORITHM AND PROGRAMS OF GRAPH GENERATION

The generation algorithm of PH_r graphs is based on the algorithms of fast generation of graphs of unbranched catacondensed hexagonal and pentagonal systems.[20,38] In the algorithm, every graph consisting of r rings is represented as two binary codes of the length r–2.

The algorithm is realized in three programs written on FORTRAN for a personal computer compatible with IBM PC XT/AT. The first program generates distributions of graphs of class PH_r according to the number of pentagonal rings and the type of symmetry. The second program generates all graphs with the given number of pentagonal rings and separates symmetrical graphs. The third program enumerates all graphs with the given vector of the ring sizes.

Generation programs primarily employ logical operations of comparison and cyclic shift of bits for integers used to code graphs. The generation process may be postponed and resumed at any stage. The algorithm and generation programs are easily modified for parallel computations.

COUNTING OF PENTAHEXAGONAL GRAPHS

The number of hexagonal systems graphs consisting of r rings is known to be defined by analytical expressions[36]

$$|H_r| = \begin{cases} \frac{1}{4}(3^{(r-2)/2}+1)^2 & \text{for } r \text{ even,} \\ \frac{1}{4}(3^{r-2} + 3^{(r-1)/2} + 3^{(r-3)/2} + 1) & \text{for } r \text{ odd.} \end{cases}$$

Numbers of mirror-symmetrical (m), centro-symmetrical (c), and unsymmetrical (u) graphs of class H_r are counted using the formulae[36]

$$m(H_r) = \begin{cases} \frac{1}{2}(3^{(r-2)/2}-1) & \text{for } r \text{ even,} \\ \frac{1}{2}(3^{(r-1)/2}-1) & \text{for } r \text{ odd,} \end{cases}$$

$$c\,(H_r) = \begin{cases} \frac{1}{2}(3^{(r-2)/2}-1) & \text{for } r \text{ even,} \\ \frac{1}{2}(3^{(r-3)/2}-1) & \text{for } r \text{ odd,} \end{cases}$$

$$u\,(H_r) = \begin{cases} \frac{1}{4}(3^{(r-2)/2}-1)^2 & \text{for } r \text{ even,} \\ \frac{1}{4}(3^{(r-2)} - 3^{(r-1)/2} - 3^{(r-3)/2} + 1) & \text{for } r \text{ odd.} \end{cases}$$

It is easily calculated that the number of graphs of pentagonal systems P_r is equal to

$$|P_r| = \begin{cases} 2^{r-4} + 2^{(r-4)/2} & \text{for } r \text{ even,} \\ 2^{r-4} + 2^{(r-5)/2} & \text{for } r \text{ odd,} \end{cases}$$

and the numbers of mirror-symmetrical, centro-symmetrical and unsymmetrical graphs are equal to

$$m\,(\mathrm{P}_r) = \begin{cases} 2^{(r-4)/2} & \text{for } r \text{ even,} \\ 2^{(r-3)/2} & \text{for } r \text{ odd,} \end{cases}$$

$$c\,(\mathrm{P}_r) = \begin{cases} 2^{(r-4)/2} & \text{for } r \text{ even,} \\ 0 & \text{for } r \text{ odd,} \end{cases}$$

$$u\,(\mathrm{P}_r) = \begin{cases} 2^{r-4} - 2^{(r-4)/2} & \text{for } r \text{ even,} \\ 2^{r-4} - 2^{(r-5)/2} & \text{for } r \text{ odd.} \end{cases}$$

Numbers of pentahexagonal systems graphs with r rings in classes S_p for $3 \le r \le 3$ are given in Table I. To generate the graphs, the IBM PC AT/286 (10 MHz) computer was used. In Table I, the generation time is given in h:m:s format for $3 \le r \le 12$. All graphs of class PH_4 are shown in Figure 2. The information about the distribution of the numbers of graphs belonging to PH_5 among the sets G_x for all the vectors of ring sizes is presented in Table II. Graphs of class PH_6 generated by vector x = (5, 6, 6, 5, 6, 5) are shown in Figure 3.

TABLE I

Distributions of graphs of pentahexagonal systems with r *ring for* $3 \le r \le 13$.

p	h	m	c	a	all
0	3	2	0	0	2
1	2	1	0	2	3
2	1	2	0	1	3
3	0	1	0	0	1
0:00:01		6	0	3	9
0	4	2	1	1	4
1	3	0	0	8	8
2	2	3	2	7	12
3	1	0	0	5	5
4	0	1	1	0	2
0:00:01		6	4	21	31
0	5	5	1	4	10
1	4	3	0	26	29
2	3	8	2	38	48
3	2	5	0	31	36
4	1	3	1	11	15
5	0	2	0	1	3
0:00:01		26	4	111	141
0	6	5	4	16	25
1	5	0	0	95	95
2	4	11	10	172	193
3	3	0	0	186	186
4	2	8	8	98	114
5	1	0	0	32	32
6	0	2	2	2	6
0:00:01		26	24	601	651
0	7	14	4	52	70
1	6	9	0	320	329
2	5	32	10	715	757
3	4	21	0	912	933
4	3	24	8	674	706
5	2	16	0	300	316
6	1	6	2	72	80
7	0	4	0	6	10
0:00:01		126	24	3051	3201
0	8	14	13	169	196
1	7	0	0	1094	1094
2	6	41	40	2815	2896
3	5	0	0	4239	4239
4	4	45	45	3870	3960
5	3	0	0	2304	2304
6	2	22	22	822	866
7	1	0	0	176	176
8	0	4	4	12	20
0:00:04		126	124	15501	15751
0	9	41	13	520	574
1	8	27	0	3632	3659
2	7	122	40	10672	10834
3	6	81	0	18387	18468
4	5	135	45	20133	20313
5	4	90	0	14697	14787
6	3	66	22	7096	7184
7	2	44	0	2194	2238
8	1	12	4	392	408
9	0	8	0	28	36
0:00:28		626	124	77751	78501

Table I (continued)

p	h	m	c	a	all
0	10	41	40	1600	1681
1	9	0	0	12029	12029
2	8	149	148	39400	39697
3	7	0	0	76788	76788
4	6	216	216	97308	97740
5	5	0	0	84672	84672
6	4	156	156	50748	51060
7	3	0	0	20928	20928
8	2	56	56	5576	5688
9	1	0	0	896	896
10	0	8	8	56	72
0:03:15		626	624	390001	391251
0	11	122	40	4840	5002
1	10	81	0	39326	39407
2	9	446	148	142405	142999
3	8	297	0	309312	309609
4	7	648	216	445716	446580
5	6	432	0	448848	449280
6	5	468	156	321744	322368
7	4	312	0	164436	164748
8	3	168	56	58640	58864
9	2	112	0	13896	14008
10	1	24	8	1968	2000
11	0	16	0	120	136
0:24:44		3126	624	1951251	1955001
0	12	122	121	14641	14884
1	11	0	0	127940	127940
2	10	527	526	506311	507364
3	9	0	0	1213785	1213785
4	8	945	945	1956420	1958310
5	7	0	0	2239488	2239488
6	6	900	900	1863396	1865196
7	5	0	0	1137888	1137888
8	4	480	480	504960	505920
9	3	0	0	159360	159360
10	2	136	136	33720	33992
11	1	0	0	4352	4352
12	0	16	16	240	272
3:08:20		3126	3124	9762501	9768751
0	13	365	121	44044	44530
1	12	243	0	413222	413465
2	11	1580	526	1775338	1777444
3	10	1053	0	4654503	4655556
4	9	2835	945	8297775	8301555
5	8	1890	0	10632249	10634139
6	7	2700	900	10070064	10073664
7	6	1800	0	7141356	7143156
8	5	1440	480	3791136	3793056
9	4	960	0	1488480	1489440
10	3	408	136	420016	420560
11	2	272	0	80632	80904
12	1	48	16	9440	9504
13	0	32	0	496	528
total		15626	3124	48818751	48837501

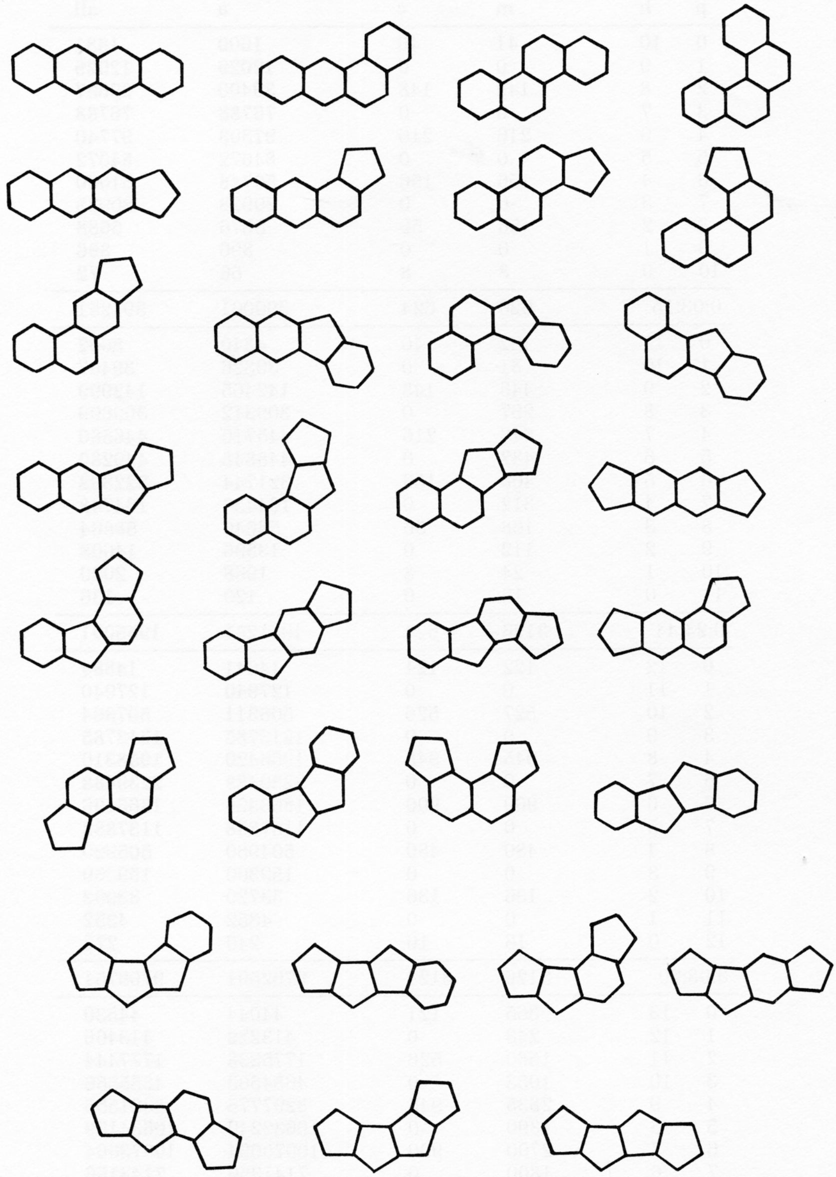

Figure 2. All pentahexagonal graphs of class PH_4.

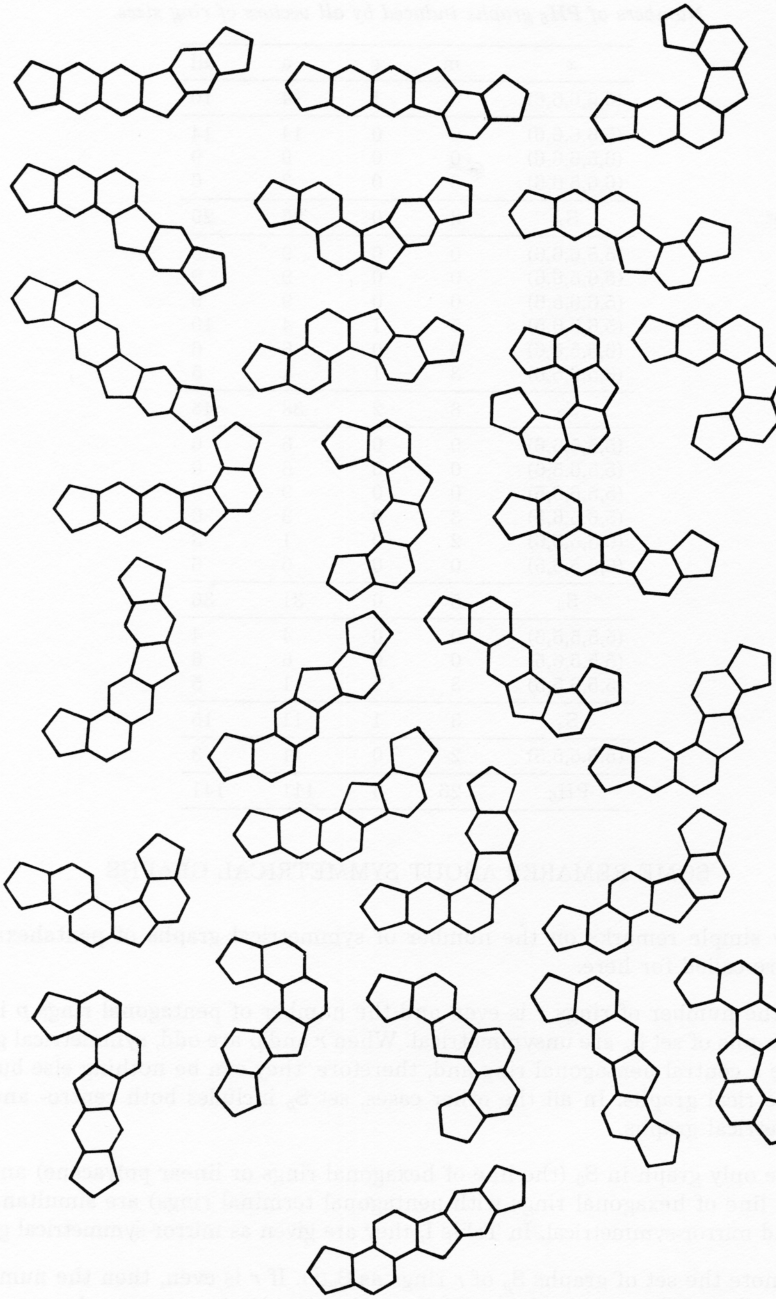

Figure 3. All graphs induced by vector $x = (5, 6, 6, 5, 6, 5)$.

TABLE II

Numbers of PH_5 graphs induced by all vectors of ring sizes.

x	m	c	a	all
(6,6,6,6,6)	5	1	4	10
(5,6,6,6,6)	0	0	14	14
(6,5,6,6,6)	0	0	9	9
(6,6,5,6,6)	3	0	3	6
S_1	3	0	26	29
(5,5,6,6,6)	0	0	9	9
(5,6,5,6,6)	0	0	9	9
(5,6,6,5,6)	0	0	9	9
(5,6,6,6,5)	5	1	4	10
(6,5,5,6,6)	0	0	6	6
(6,5,6,5,6)	3	1	1	5
S_2	8	2	38	48
(5,5,5,6,6)	0	0	6	6
(5,5,6,5,6)	0	0	6	6
(5,5,6,6,5)	0	0	9	9
(5,6,5,6,5)	3	0	3	6
(6,5,5,5,6)	2	0	1	3
(6,5,5,6,5)	0	0	6	6
S_3	5	0	31	36
(5,5,5,5,6)	0	0	4	4
(5,5,5,6,5)	0	0	6	6
(5,5,6,5,5)	3	1	1	5
S_4	3	1	11	15
(5,5,5,5,5)	2	0	1	3
PH_5	26	4	111	141

SOME REMARKS ABOUT SYMMETRICAL GRAPHS

A few simple remarks on the number of symmetrical graphs of pentahexagonal systems are called for here.

1) If the number of rings r is even and the number of pentagonal rings p is odd, then all graphs of set S_p are unsymmetrical. When r and p are odd, symmetrical graphs in S_p have a central pentagonal ring and, therefore, they can be nothing else but mirror-symmetrical graphs. In all the other cases, set S_p includes both centro- and mirror-symmetrical graphs.

2) The only graph in S_0 (the line of hexagonal rings or linear polyacene) and that in S_2 (the line of hexagonal rings with pentagonal terminal rings) are simultaneously centro- and mirror-symmetrical. In Table I, they are given as mirror-symmetrical graphs.

3) Denote the set of graphs S_p of r rings as $S_p(r)$. If r is even, then the number of centro-symmetrical graphs in $S_p(r)$ and $S_p(r+1)$ coincides for every p. A new central hexagonal ring may be added to each centro-symmetrical graph of $S_p(r)$ without loss of symmetry. It is obvious that $|S_p(r)| = |S_p(r+1)| = 0$ for odd p.

4) Consider the set of mirror-symmetrical graphs. Let the number of rings r be even. If p is odd, then $|S_p(r)| = 0$. If p is even, then $|S_p(r)| = |S_p(r-1)| + |S_{p+1}(r-1)|$ or $|S_p(r)| = (|S_{p+1}(r+1)| + b)/2$, where $b=1$ for $p=0,2$ and $b=0$ otherwise. Let the number of rings r be odd. If p is even, then $|S_p(r)| = |S_{p+1}(r)| + |S_p(r-1)|$ or $|S_p(r)| = 3|S_p(r-1)| - b$. In order to check these equalities we have to add a new central pentagonal or hexagonal ring to the relevant graphs.

5) Let the vector of the graph ring sizes contain two terminal pentagonal rings, $x = (5,6,6,\cdots,6,6,5)$. Since the terminal rings have no effect on adding other rings, so $|G_x| = |H_r|$, $m(G_x) = m(H_r)$, $c(G_x) = c(H_r)$, $a(G_x) = a(H_r)$. It is clear that this property is valid for terminal rings of arbitrary size.

6) Let vector x contain only the pentagonal terminal ring $x = (5,6,6,\cdots,6)$, *i.e.* all graphs in G_x are unsymmetrical. Each unsymmetrical graph of class H_r generates two graphs of class G_x by substituting a pentagonal ring for each hexagonal terminal one, while a symmetrical graph generates only the graph of G_x. Therefore, $|G_x| = 2a(H_r) + m(H_r) + c(H_r)$.

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SAŽETAK

Generiranje grafova nerazgranatih pentaheksagonskih katakondeziranih sustava

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Razmatrano je prebrojavanje grafova nerazgranatih pentaheksagonskih katakondenziranih sustava. Tipičan graf te klase jest vrpca složena od međusobno povezanih petero- i šesteročlanih prstenova. Prebrojani su svi takovi grafovi sa 3 do 13 prstenova.