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Isomers of Polycyclic Conjugated Hydrocarbons with Six-Membered and Seven-Membered Rings

B. N. Cyvin, S. J. Cyvin*, and J. Brunvoll

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

Summary. Monoheptapolyhexes are polygonal systems with exactly one heptagon and otherwise hexagons. General formulations with emphasis on the C_nH_s formula, and the first enumerations of C_nH_s isomers are reported for these systems. Also a more general class of systems is treated in some detail, viz. $P_{7(6)}$, which consists of hexagons and/or heptagons. The maximum numbers of heptagons for given C_nH_s formulas are studied, and the possible C_nH_s formulas are specified.

Keywords. Polycyclic conjugated hydrocarbon; Monoheptapolyhex; Isomer enumeration; Heptagonal/hexagonal rings.

Isomere von polycyclischen konjugierten Kohlenwasserstoffen mit 6- und 7-gliedrigen Ringen

Zusammenfassung. „Monoheptapolyhexe" sind polygonale Systeme mit genau einem Siebeneck und ansonsten nur Sechsecken. Es wird der allgemeine Formelapparat mit Betonung auf C_nH_s und die Auswertung bezüglich der Anzahl von C_nH_s-Isomeren für diese Systeme berichtet. Ebenso wird über eine generellere Klasse von Systemen, nämlich $P_{7(6)}$ berichtet, die aus Sechsecken und/oder Siebenecken besteht. Die Maximalanzahl von Siebenecken für gegebene C_nH_s-Formeln wird untersucht und mögliche C_nH_s-Formeln werden angegeben.

Introduction

The completely condensed polycyclic conjugated hydrocarbons are of great interest in organic chemistry. As chemical graphs [1] they are represented by *polygonal systems*, viz. connected geometrical constructions of polygons, where any two polygons either share exactly one edge or are disjoint. Benzenoid hydrocarbons [2, 3] possess exclusively six-membered rings and are represented by benzenoid systems [3–5]. Dias [6] has listed chemically known polycyclic conjugated hydrocarbons with different ring sizes. In some of his theoretical analyses he concentrated upon structures with one ring size in addition to six-membered rings. A special kind of such hydrocarbons are represented as chemical graphs by the *mono-q-polyhexes* [7]. A mono-q-polyhex is a polygonal system consisting of exactly one q-gon and otherwise hexagons (if any). Benzenoids [8], fluoranthenoids [9, 10] and biphenylenoids [11] are mono-q-polyhexes with $q = 6$, 5 and 4, respectively. Some of the cited works [8, 9, 11] contain more or less extensive enumerations of C_nH_s isomers of the systems in question. It appears that many of the topological properties

of mono-q-polyhexes are substantially different for $q < 6$ and $q > 6$, as might be expected. In the present work the first (extensive) enumerations of mono-q-polyhexes with $q > 6$ are reported; here the monoheptapolyhexes ($q = 7$) are treated. Furthermore, some theoretical studies on polygonal systems with hexagons and/or heptagons are performed. Here the number of heptagons may be more than one.

Definitions and Notation

A classification of polygonal systems (see above for a definition) to be employed here, is closely connected with the classification of polyhexes which was adopted in a recent review [12]. Presently we shall only consider simply connected polygonal systems. They can only have vertices of degree three or two, the latter kind only found on the perimeter. A benzenoid is a simply connected, geometrically planar (non-helicenic) polyhex. Correspondingly, a simply connected, geometrically planar mono-q-polyhex (see above) may be termed a *mono-q-benzenoid*. Notice that a mono-q-benzenoid with $q = 6$ is a benzenoid. A simply connected, geometrically nonplanar (helicenic) mono-q-polyhex may be referred to as a *mono-q-helicene*; for $q = 6$ it is a helicene. The mono-q-henzenoids and mono-q-helicenes taken together constitute the class of *mono-q-fusenes*.

Let r be used to designate the number of polygons (or rings) of a polygonal system, P. Another important invariant of P is n_i, the number of internal vertices. An internal vertex is defined as a vertex shared by three polygons. A polygonal system is *catacondensed* when it does not possess any internal vertex ($n_i = 0$), while a *pericondensed* polygonal system has at least one internal vertex ($n_i > 0$).

A polygonal system (P) corresponds to a hydrocarbon with a formula C_nH_s. Here n, the number of carbon atoms, indicates the total number of vertices in P. The number of hydrogens, s, is at the same time the number of secondary carbon atoms and corresponds to the number of vertices of degree two in P.

Mono-q-Polyhexes

Let r_q be used to designate the number of q-gons in a polygonal system. Then a mono-q-polyhex is characterized by $r = r_6 + r_q$ where $r_q = 1$, and we shall introduce $r_6 = h$ (the number of hexagons).

For a simply connected mono-q-polyhex (mono-q-fusene) one has the following relations between four of the invariants which were introduced above.

$$h = \tfrac{1}{2}(n - s), \quad n_i = n - 2s + q \tag{1}$$

$$n = 4h - n_i + q, \quad s = 2h - n_i + q \tag{2}$$

Notice also that $r = h + 1$.

Monoheptapolyhexes

General Formulations

The formulations of the preceding section are applicable to monoheptapolyhexes (mono-7-polyhexes) with $q = 7$.

The maximum number of internal vertices, $(n_i)_{max}$, for mono-q-fusenes at a given h is of interest. One of the present authors [7] conjectured an expression for $(n_i)_{max}$, which later was assumed to be valid for $q = 3$, 4, 5 (and 6) [11]. However, the conjecture was disproved for $q > 6$ [13]. Instead, we propose the following relations:

$$0 \leqslant n_i \leqslant 2h + 3 - \lceil (12h + 9)^{1/2} \rceil. \tag{3}$$

These bounds are simply identical to those of benzenoids with $h + 1$ hexagons [8]. In other words, it is inferred that $(n_i)_{max}$, the upper bound in Eq. (3), for a mono-q-fusene ($q > 6$) with r polygons is the same as $(n_i)_{max}$ for a benzenoid with r polygons (which are hexagons). A mono-q-fusene with $n_i = (n_i)_{max}$ is certainly non-helicenic and therefore a mono-q-benzenoid. It is referred to as an *extremal* mono-q-benzenoid in analogy with the class of extremal benzenoids [8, 14–18].

From Eqs. (2) and (3) one finds the coefficients of the formulas of extremal monoheptabenzenoids, say n^a and s^a as

$$n^a = 2h + 4 + \lceil (12h + 9)^{1/2} \rceil, \quad s^a = 4 + \lceil (12h + 9)^{1/2} \rceil. \tag{4}$$

Hence $n^a = s^a + 2h$. Here $h = 0, 1, 2, \ldots$.

A one-to-one correspondence may be established between all the possible C_nH_s monoheptabenzenoid or monoheptafusene formulas (which amounts to the same) on one hand, and the C_NH_S benzenoid formulas on the other. Any C_NH_S benzenoid isomer can namely be converted to a C_nH_s monoheptabenzenoid isomer by expanding one of the hexagons at the perimeter to a heptagon. Then $n = N + 1$ and $s = S + 1$ is valid. Furthermore, it is inferred that this conversion $C_NH_S \rightarrow C_nH_s$ accounts for all the possible monoheptabenzenoid formulas. In consequence, the C_nH_s formulas for catacondensed monoheptabenzenoids (where $n = 2s - 7$) are nonbenzenoid formulas, while the C_NH_S formulas of extremal benzenoids [8] are not compatible with the monoheptabenzenoids. Otherwise the formulas of benzenoids and monoheptabenzenoids overlap.

For a given n, which C_nH_s formulas are possible for the monoheptabenzenoids? The corresponding question for benzenoids has been answered [8]. Then, by virtue of the above discussion it was found:

$$2\lceil \tfrac{1}{2}(n-1) + \tfrac{1}{2}(6n-6)^{1/2} \rceil - n + 2 \leqslant s \leqslant n + 2 - 2\lceil \tfrac{1}{4}(n-3) \rceil. \tag{5}$$

Here the possible values of n are $n = 7$, 11, 14, 15, 17, 18, 19,... (not 8, 12, 13, 16). In consequence, $s = 7$, 9, 10, 11,... (not 8). For a given n (in the allowed domain), all the s values between the upper and lower bounds on Eq. (5) inclusive are realized, provided that the parities of n and s are taken into account: either both n and s are even, or both of them are odd.

Isomer Enumeration

A computer program was designed in order to generate the monoheptabenzenoid C_nH_s isomers successively with increasing h values. A complete listing of the numbers of isomers for $h \leqslant 7$ is given in Table 1, while Table 2 shows incomplete data for higher h values, but so that the extremal systems for every h are included. A special algorithm was used to recognize the symmetry of the generated systems; in general the possible symmetry groups are D_{7h}, C_{7h}, C_{2v} and C_s. In Tables 1 and 2 there are

Table 1. Numbers of C_nH_s isomers of simply connected, geometrically planar monoheptapolyhexes (monoheptabenzenoids): complete data for $h \leqslant 7$

h	n_i	Formula	D_{7h}	C_{2v}	C_s	Total
0	0	C_7H_7	1	0	0	1
1	0	$C_{11}H_9$	0	1	0	1
2	0	$C_{15}H_{11}$	0	3	1	4
	1	$C_{14}H_{10}$	0	1	0	1
3	0	$C_{19}H_{13}$	0	3	10	13
	1	$C_{18}H_{12}$	0	1	4	5
	2	$C_{17}H_{11}$	0	2	0	2
4	0	$C_{23}H_{15}$	0	9	47	56
	1	$C_{22}H_{14}$	0	4	28	32
	2	$C_{21}H_{13}$	0	4	8	12
	3	$C_{20}H_{12}$	0	1	2	3
5	0	$C_{27}H_{17}$	0	10	221	231
	1	$C_{26}H_{16}$	0	4	174	178
	2	$C_{25}H_{15}$	0	8	74	82
	3	$C_{24}H_{14}$	0	3	23	26
	4	$C_{23}H_{13}$	0	4	5	9
6	0	$C_{31}H_{19}$	0	29	970	999
	1	$C_{30}H_{18}$	0	14	942	956
	2	$C_{29}H_{17}$	0	21	522	543
	3	$C_{28}H_{16}$	0	8	196	204
	4	$C_{27}H_{15}$	0	7	67	74
	5	$C_{26}H_{14}$	0	2	17	19
	6	$C_{25}H_{13}$	0	1	0	1
7	0	$C_{35}H_{21}$	0	35	4241	4276
	1	$C_{34}H_{20}$	0	14	4891	4905
	2	$C_{33}H_{19}$	0	35	3255	3290
	3	$C_{32}H_{18}$	0	18	1461	1479
	4	$C_{31}H_{17}$	0	20	580	600
	5	$C_{30}H_{16}$	0	3	190	193
	6	$C_{29}H_{15}$	0	9	44	53
	7	$C_{28}H_{14}$	1	1	3	5

no entries for C_{7h} because the smallest monoheptabenzenoids with this symmetry have $h = 21$.

The invariants of Tables 1 and 2, which include the C_nH_s formulas, were generated automatically as an "empirical" material. It is gratifying to observe that this material is completely consistent with Eqs. (3)–(5) and with the discussions attached to these equations. This is a strong indication that the above theory is correct.

Table 2. Numbers of C_nH_s isomers of simply connected, geometrically planar monoheptapolyhexes (monoheptabenzenoids): incomplete data for $h > 7$

h	n_i	Formula	C_{2v}	C_s	Total
8	5	$C_{34}H_{18}$	15	1677	1692
	6	$C_{33}H_{17}$	16	528	544
	7	$C_{32}H_{16}$	7	128	135
	8	$C_{31}H_{15}$	5	16	21
9	7	$C_{36}H_{18}$	15	1457	1472
	8	$C_{35}H_{17}$	18	388	406
	9	$C_{34}H_{16}$	6	66	72
	10	$C_{33}H_{15}$	2	1	3
10	9	$C_{38}H_{18}$	20	1186	1206
	10	$C_{37}H_{17}$	18	222	240
	11	$C_{36}H_{16}$	1	18	19
11	11	$C_{40}H_{18}$	16	735	751
	12	$C_{39}H_{17}$	9	99	108
	13	$C_{38}H_{16}$	1	1	2
12	13	$C_{42}H_{18}$	8	420	428
	14	$C_{41}H_{17}$	6	20	26
13	15	$C_{44}H_{18}$	8	160	168
	16	$C_{43}H_{17}$	1	2	3
14	17	$C_{46}H_{18}$	3	38	41
15	19	$C_{48}H_{18}$	1	5	6

Polygonal Systems with Hexagons and/or Other Polygons of a Given Size

The systems considered here are simply connected polygonal systems, $P_{q(6)}$, which consist of hexagons and/or q-gons. They are characterized by

$$r = r_6 + r_q \tag{6}$$

where $r_6 \geqslant 0$, $r_q > 0$. The mono-q-fusenes are special cases for $r_q = 1$.

For a simply connected polygonal system it is easily found [19, 20]

$$\Sigma q = n + 2r + n_i - 2 \tag{7}$$

where Σq is the polygon-edge sum, in the present case for $P_{q(6)}$:

$$\Sigma q = 6r_6 + qr_q. \tag{8}$$

On combining Eqs. (6)–(8) it is obtained

$$6r + (q-6)r_q = n + 2r + n_i - 2. \tag{9}$$

Isomers of a given C_nH_s formula are considered; hence the n and r values are fixed, and in particular:

$$r = \tfrac{1}{2}(n-s) + 1. \tag{10}$$

The symbol n_i in Eq. (9) indicates the number of internal vertices in $P_{q(6)}$. Consider now a benzenoid ($r = r_6$) with the given formula (C_nH_s), if it exists. Then clearly

$$6r = n + 2r + n_i^* - 2 \tag{11}$$

where n_i^* is the number of internal vertices in the benzenoid under consideration. On subtracting (11) from (9) it is obtained

$$(q-6)r_q = n_i - n_i^*. \tag{12}$$

Even if C_nH_s is a formula for which no benzenoid can be constructed (a nonbenzenoid formula), Eq. (12) can be applied. One should only interpret n_i^* as

$$n_i^* = n - 2s + 6. \tag{13}$$

Polygonal Systems with Hexagons and/or Heptagons

Let a simply connected polygonal system be identified by the symbol $P_{7(6)}$ when it consists of hexagons and/or heptagons. This is the special case for $q = 7$ of the class which was considered in the preceding section. In consequence, a $P_{7(6)}$ system is characterized by $r = r_6 + r_7$, where $r_6 \geqslant 0$, $r_7 > 0$. The monoheptafusenes are special cases for $r_7 = 1$.

Maximum Number of Heptagons

Consider the $P_{7(6)}$ systems with a given formula C_nH_s. What is the maximum number of heptagons, $(r_7)_{max}$, compatible with that formula? This is an interesting question, which was first posed by Dias [21]. However, he did not give a satisfactory answer [6, 21, 22]; in the following we shall demonstrate counterexamples to some of his conclusions.

On inserting $q = 7$ one obtains from Eqs. (12) and (13):

$$r_7 = n_i - n_i^* = n_i - n + 2s - 6. \tag{14}$$

It is clear from this relation that the maximum of r_7 is achieved on maximizing n_i. The formula C_nH_s is associated with a definite total number of polygons, r; cf. Eq. (10). Now $(n_i)_{max}$ for a given r clearly cannot exceed the maximum number of internal vertices for a benzenoid with r hexagons. On inserting from (10) into the known expression for this maximum value [8], one obtains

$$n_i \leqslant n - s + 3 - \lceil (6n - 6s + 9)^{1/2} \rceil \tag{15}$$

and consequently:

$$r_7 \leqslant s - 3 - \lceil (6n - 6s + 9)^{1/2} \rceil. \tag{16}$$

This relation holds also if C_nH_s is a nonbenzenoid formula. If the sign of equality in (16) can be realized for a $P_{7(6)}$ isomer with the formula C_nH_s, then $r_7 = (r_7)_{max}$ for this formula. In the serach for such an isomer one knows the total number of polygons (r) from Eq. (11), while the number of internal vertices is

$$n_i = r_7 + n_i^* = r_7 + n - 2s + 6 \tag{17}$$

in accordance with Eq. (14). It may happen that

$$s - 3 - \lceil (6n - 6s + 9)^{1/2} \rceil > \tfrac{1}{2}(n - s) + 1. \tag{18}$$

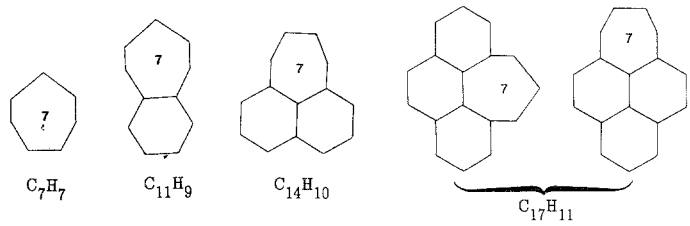
In that case

$$r_7 \leqslant \tfrac{1}{2}(n - s) + 1 \tag{19}$$

is a sharper upper bound than (16). If the sign of equality in (19) is realized, then $r_7 = r$, which means that the $P_{7(6)}$ system consists exclusively of heptagons.

As the first examples, consider the monoheptabenzenoids of Fig. 1. In all these cases, Eq. (16) gives $r_7 \leqslant 1$. Therefore these systems possess the maximum numbers of heptagons for the formula in question; $r_7 = (r_7)_{\max} = 1$. More advanced examples are illustrated in Fig. 2: the maximum numbers of heptagons for $P_{7(6)}$ systems with the three formulas therein are again consistent with Eq. (16), where the sign of equality is realized in all three cases. Analyses of Dias imply $(r_7)_{\max} = 1$ for $C_{26}H_{14}$ [22], $(r_7)_{\max} = 1$ for $C_{34}H_{16}$ [22] and $(r_7)_{\max} = 3$ for $C_{34}H_{18}$ [6]. Hence the three systems of Fig. 2 are counterexamples to the Dias' statements.

Consider now $P_{7(6)}$ systems where, in contrast to those of Figs. 1 and 2, the heptagons are predominant. In the cases $C_{22}H_{16}$ and $C_{21}H_{15}$ (see Fig. 3) Eq. (16) gives $r_7 \leqslant 6$ and $r_7 \leqslant 5$, respectively. In both cases the condition (18) is satisfied so



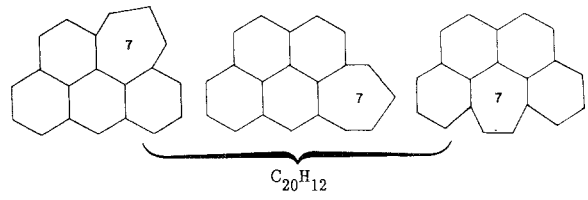


Fig. 1. All extremal monoheptabenzenoids for $h \leqslant 4$; they all have $r_7 = (r_7)_{\max} = 1$; here and in the following figures, inscribed numerals indicate polygon dimensions

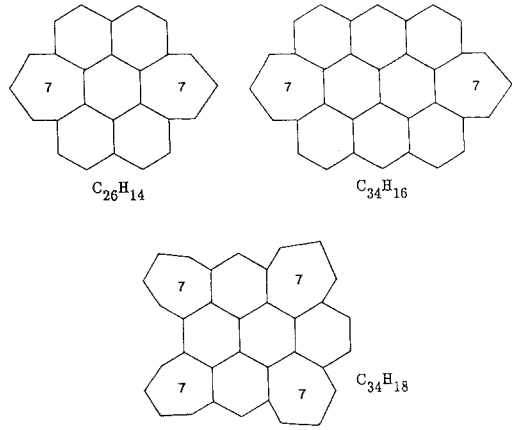


Fig. 2. Three $P_{7(6)}$ systems with $r_7 = (r_7)_{\max}$ for the given formulas

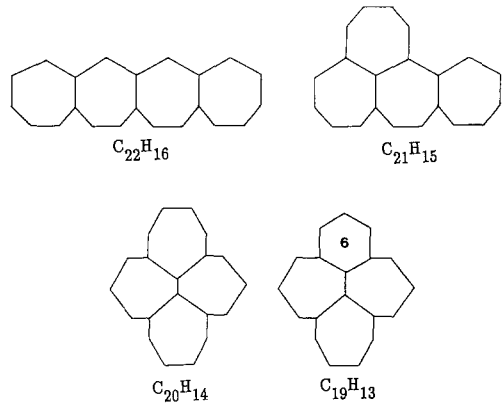


Fig. 3. Four $P_{7(6)}$ systems with $r = 4$ and $r_7 = (r_7)_{max}$

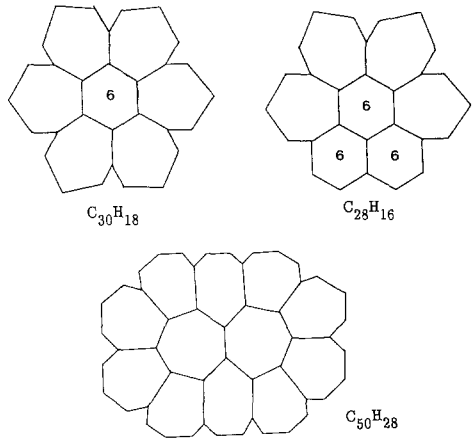


Fig. 4. Three $P_{7(6)}$ systems with $r_7 = (r_7)_{max}$

that (19) comes into operation; it yields $r_7 \leqslant 4$ in both cases. The examples in Fig. 3 show that, indeed, $r = r_7 = 4$ (only heptagons) is realized in these two cases. This last feature is also realized for $C_{20}H_{14}$ (Fig. 3), for which both (16) and (19) give $r_7 \leqslant 4$. On the other hand, Eq. (16) gives $r_7 \leqslant 3$ for $C_{19}H_{13}$, the last example in Fig. 3, so that no system with only heptagons is possible for this formula. The three systems in Fig. 4 are counterexamples to Dias [6], from whose analysis the values $(r_7)_{max} = 5$, 3 and 10 are prescribed for $C_{30}H_{18}$, $C_{28}H_{16}$ and $C_{50}H_{28}$, respectively. The systems in Fig. 4 are again consistent with our relations (16) and (19).

For the sake of completeness we should also demonstrate cases where the sign of equality in (16) cannot be realized. Consider the first the "normal" case of $r = 10$ for $C_{40}H_{22}$ (see Fig. 5). Here Eq. (16) gives $r_7 \leqslant 8$, and $r_7 = (r_7)_{max} = 8$ ($n_i = 10$), is realized. On the other hand, for $C_{41}H_{23}$, which also is compatible with $r = 10$, Eq. (16) gives $r_7 \leqslant 9$. If the sign of equality could be realized here, one should have $r_7 = 9$, $n_i = 10$. It seems impossible to construct such a system; we believe that $(r_7)_{max} = 8$ is valid in this case. Two examples of $C_{41}H_{23}$ systems with $r_7 = 8$ ($n_i = 9$) are displayed in Fig. 5. Similarly, for $C_{42}H_{24}$ ($r = 10$) one has $r_7 \leqslant 10$ from (16), but $r_7 = 10$, $n_i = 10$ can clearly not be realized for a system with only heptagons (see below). Here one has $(r_7)_{max} = 9$; two systems with $r_7 = 9$ ($n_i = 9$) are included in Fig. 5. If we proceed to $C_{43}H_{25}$ ($r = 10$) we find in the "normal" way that systems with $r_7 = (r_7)_{max} = 10$ (only heptagons) and $n_i = 9$ easily can be constructed.

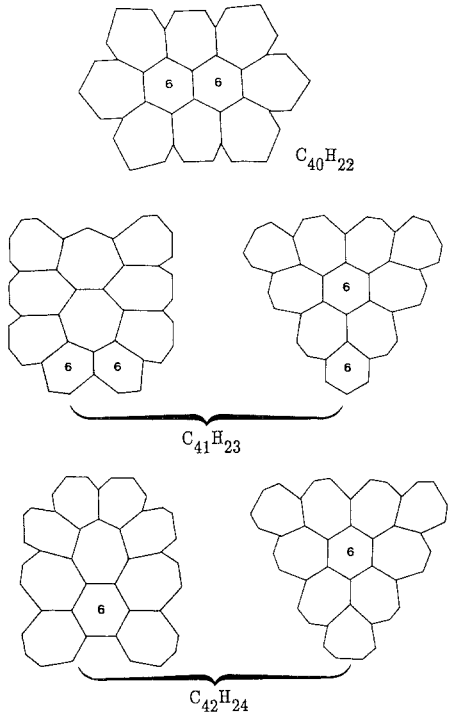


Fig. 5. Some $P_{7(6)}$ systems with $r = 10$ and (presumably) $r_7 = (r_7)_{max}$

Possible Chemical Formulas

Which C_nH_s formulas are possible for $P_{7(6)}$? This question was posed by Dias and supposed to be answered by his Table PAH_7 [6]. We found some errors in this table and therefore give an improved version in Fig. 6. Only even-carbon C_nH_s formulas are considered herein (as in Dias' Table PAH_7) since these are the formulas of particular interest for chemists. The above question may be answered in general (for both even- and odd-carbon C_nH_s formulas) by relations similar to Eq. (5) for monoheptapolyhexes.

As a matter of fact, the lower bounds of s for given n values in the $P_{7(6)}$ systems are realized in monoheptapolyhexes, so that

$$s \geqslant 2\lceil \tfrac{1}{2}(n-1) + \tfrac{1}{2}(6n-6)^{1/2} \rceil - n + 2 \tag{20}$$

is valid. But for $P_{7(6)}$ systems in general also $n = 12$ is possible. In this case Eq. (20) reproduces the formula $C_{12}H_{10}$ ($r = r_7 = 2$; two heptagons). For $n = 38$, 48 and 60, Eq. (20) prescribes $C_{38}H_{16}$, $C_{48}H_{18}$ and $C_{60}H_{20}$ for the respective formulas with minimum s values see Fig. 7. These formulas should not exist for $P_{7(6)}$ according to Dias (Table PAH_7 [6]).

The upper bound of s as a function of n is different from the one of Eq. (5) for $P_{7(6)}$ systems in general. In Fig. 6 the heavy line indicates the upper bound of s for monoheptapolyhexes. In order to find this upper bound for $P_{7(6)}$, it is first observed that

$$n = 13 + 5i + j, \quad s_{max} = 9 + 3i + j \tag{21}$$

for $i = 0, 1, 2, \ldots$, and $j = 0, 1, 2, 3, 4$. This scheme incorporates $C_{13}H_9$, which is a benzenoid formula, but applies to $r = r_6 + r_7$ only for $r_7 = 0$. However, the formulas

n	s										
12	10										
14	10										
16	12										
18	12										
20	12	14									
22	14	16									
24	14	16									
26	14	16	18								
28	14	16	18								
30	16	18	20								
32	16	18	20	22							
34	16	18	20	22							
36	16	18	20	22	24						
38	16	18	20	22	24						
40	18	20	22	24	26						
42	18	20	22	24	26	28					
44	18	20	22	24	26	28					
46	18	20	22	24	26	28	30				
48	18	20	22	24	26	28	30				
50	20	22	24	26	28	30	32				
52	20	22	24	26	28	30	32	34			
54	20	22	24	26	28	30	32	34			
56	20	22	24	26	28	30	32	34	36		
58	20	22	24	26	28	30	32	34	36		
60	20	22	24	26	28	30	32	34	36	38	
62	22	24	26	28	30	32	34	36	38	40	
64	22	24	26	28	30	32	34	36	38	40	
66	22	24	26	28	30	32	34	36	38	40	42
68	22	24	26	28	30	32	34	36	38	40	42

C_nH_s

Fig. 6. Possible even-carbon formulas for $P_{7(6)}$ systems when $n \leqslant 68$

C_7H_7, $C_{11}H_9$ and $C_{12}H_{10}$ for $P_{7(6)}$ systems are not covered. In (21),

$$i = \lfloor (n-13)/5 \rfloor = \lfloor (n-3)/5 \rfloor - 2. \tag{22}$$

This expression was inserted into n of Eq. (21), whereupon it was obtained

$$j = n - 3 - 5\lfloor (n-3)/5 \rfloor. \tag{23}$$

As the final step, the expressions from (22) and (23) were inserted in s_{max} of Eq. (21) and yielded:

$$s \leqslant n - 2\lfloor (n-3)/5 \rfloor. \tag{24}$$

This upper bound is realized as s_{max} for every possible n, also for $n = 7$, 11 and 12. Furthermore, we find all the upper bounds of s in Table PAH_7 of Dias [6] to be reproduced by Eq. (24).

Conclusion

Dias [6] has documented the chemical importance of polycyclic conjugated hydrocarbons with one ring size in addition to six-membered rings. In the present work such systems with six-membered and/or seven-membered rings are treated, as represented by the polygonal systems $P_{7(6)}$. During this work several inaccuracies

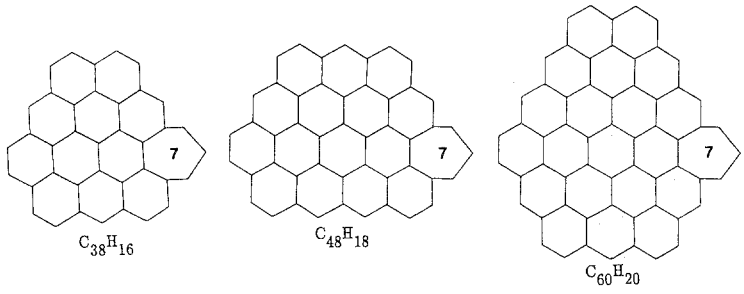


Fig. 7. Monoheptapolyhexes (special $P_{7(6)}$ systems) where $s = s_{min}$ for the pertinent n values in C_nH_s

and errors in the book of Dias [6] were detected. Since this is a frequently cited and widely used handbook it is important that errors therein are corrected. In particular, we have pointed out Dias' [6] unsatisfactory treatment of $(r_7)_{max}$ for $P_{7(6)}$ systems. But there are also inaccuracies and wrong conclusions in Dias' treatment of $(r_q)_{max}$ for $P_{q(6)}$ systems when $q = 3, 4, 5, 8, 9$ or 10. Furthermore, we have pointed out some few errors in Dias' [6] Table PAH_7 for the possible C_nH_s formulas of $P_{7(6)}$ systems. Some errors were also detected in Dias' Tables PAH_8 and PAH_9, and more significant errors in each of Tables PAH_3, PAH_4 and PAH_5. A detailed specification of errors in the Handbook of Dias [6], supported by counterexamples, is available on request to the authors.

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References

[1] Trinajstić N. (1992) Chemical Graph Theory, 2nd edn. CRC Press, Boca Raton
[2] Clar E. (1964) Polycyclic Hydrocarbons, Vols. 1, 2. Academic Press, London
[3] Gutman I., Cyvin S. J. (1989) Introduction to the Theory of Benzenoid Hydrocarbons. Springer, Berlin Heidelberg New York Tokyo
[4] Gutman I. (1982) Bull. Soc. Chim. Beograd **47**: 453
[5] Cyvin S. J., Gutman I. (1988) Kekulé Structures in Benzenoid Hydrocarbons. Springer, Berlin Heidelberg New York Tokyo (Lecture Notes in Chemistry, Vol. 46)
[6] Dias J. R. (1988) Handbook of Polycyclic Hydrocarbons, Part B. Elsevier, Amsterdam
[7] Cyvin S. J. (1992) J. Math. Chem. **9**: 389
[8] Brunvoll J., Cyvin B. N., Cyvin S. J. (1992) Topics Current Chem. **162**: 181
[9] Dias J. R. (1991) Chem. Phys. Letters **185**: 10
[10] Cyvin S. J. (1992) J. Mol. Struct. (Theochem) **262**: 219
[11] Cyvin S. J., Cyvin B. N., Brunvoll J. (1993) Chem. Phys. Letters **201**: 273
[12] Cyvin B. N., Brunvoll J., Cyvin S. J. (1992) Topics Current Chem. **162**: 65
[13] Lloyd E. K. (submitted) J. Math. Chem.
[14] Cyvin S. J., Brunvoll J., Cyvin B. N. (1991) Match (Mülheim) **26**: 27
[15] Cyvin S. J., Cyvin B. N., Brunvoll J. (1993) Topics Current Chem. **166**: 65
[16] Cyvin S. J., Brunvoll J., Cyvin B. N. (1991) J. Serb. Chem. Soc. **56**: 369

[17] Cyvin S. J., Cyvin B. N., Brunvoll J., Gutman I., John P. E. (1993) J. Serb. Chem. Soc. **58**: 1
[18] Cyvin S. J., Cyvin B. N., Brunvoll J. (1993) Monatsh. Chem. **124**: 477
[19] Cyvin S. J., Brunvoll J., Cyvin B. N. (1993) Chem. Phys. Lett. **205**: 343
[20] Brunvoll J., Cyvin B. N., Cyvin S. J. (1993) Computers and Chemistry **17**: 291
[21] Dias J. R. (1982) J. Chem. Inf. Comput. Sci. **22**: 139
[22] Dias J. R. (1983) Match (Mülheim) **14**: 83

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