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Constant-isomer benzenoid series and their topological characteristics

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Summary. New constant-isomer series are presented. Two classes of constant-isomer series based on the topological correspondence of their member benzenoids are identified. The isomer numbers for the constant-isomer series alternate between singlet and doublet occurrence. Constant-isomer series with the same isomer number possess a pairwise one-to-one topological correspondence between their benzenoid membership. A correspondence also exists between threefold monoradical and diradical benzenoids belonging to these constant-isomer series. These topological relationships represent a new paradigm that we ascribe as an edge effect of our periodic table for benzenoids.

Key words: Benzenoids – Enumeration – Topological characteristics – Periodic table – Symmetry group

Introduction

Our previous work demonstrated how the formula periodic table for benzenoid hydrocarbons (Table PAH6) could be used to derive graphical invariants like the sixth coefficient (a_6) of the characteristic polynomial [1, 2]. Table PAH6 has also provided the framework for benzenoid enumeration [3, 4]. It is well known that as the number of carbons increases the number alkane isomers increases [5]. In contrast, this table led us to identify special benzenoid series for which the number of isomers remains constant as the number of carbons increases [4, 6, 7]. In this paper, new results concerning constant-isomer benzenoid series and their topological characteristics are presented. These constant-isomer benzenoid series constitute a phenomenon that we call an edge effect of Table PAH6 that is

Table 1. Glossary of terms

d_s	net tree disconnections of internal graph edges (positive values) or connections (negative value—called negative disconnection)
N_c	total number of carbon atoms in a PAH
N_H	total number of hydrogen atoms in a PAH
N_{Ic}	number of internal carbon atoms in a PAH having a degree of 3
N_{Pc}	number of peripheral carbon atoms in a PAH having a degree of 3
PAH6	polycyclic aromatic hydrocarbon containing exclusively fused hexagonal rings; also referred to as benzenoid and polyhex
$\|P\| = p = N_c$	total number of graph points
p_3	number of graph points (vertices) having a degree of 3
$\|Q\| = q$	number of graph edges (lines or C–C bonds)
q_I	number of internal graph edges
q_p	number of peripheral graph edges
r	number of rings

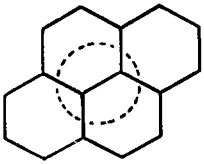
intricately related to the topology of the benzenoid members. Herein, we claim to have identified a new paradigm that may have universal topological implications since the polyhex structure is fundamental to nature.

A *periodic table set* is defined as a partially ordered set (poset) forming a two-dimensional array which complies with the *triad principle* where a central element has a metric property that is the arithmetic mean of two adjacent surrounding member elements. Both the periodic table of elements and Table PAH6 are sets that obey this definition. Key features of this definition are hierarchal ordering, two-dimensionality, and edge effects. By edge effect we mean that set members located on the edge or two-dimensional boundary possess properties that are more exceptional relative to the other set members. In Table PAH6, overall or average properties associated with isomer groups (e.g., $\bar{E}_\pi$) assume a hierarchal ordering. Similarly, in the periodic table of elements, the overall or average properties belonging to isotope groups assume a hierarchal ordering. These tables constitute partially ordered sets $X = (X, \leqslant)$ since their properties (x, y) satisfy the mathematical conditions of reflexivity $(x \leqslant x)$, antisymmetry $(x \leqslant y$ and $y \leqslant x \rightarrow x = y)$, and transitivity $(x \leqslant y$ and $y \leqslant z \rightarrow x \leqslant z)$.

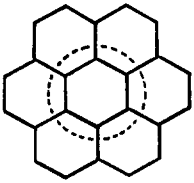
The polyhex graphs considered in this work are totally isomorphic to real benzenoids. Strictly peri-condensed benzenoids have no cata-condensed appendages and a minimal number of bay regions. This translates to a group of benzenoids without helicenic components and are, therefore, incapable of exhibiting stereoisomers characteristic of helicenes. It is believed that these strictly peri-condensed benzenoids represent the most probable constituents of carbonaceous materials.

Strictly peri-condensed benzenoids and their excised internal structures

Throughout this paper only the σ-bond molecular graph (polyhex graph) will be shown for all benzenoid hydrocarbons where the carbon and hydrogen atoms and the C—H and $p\pi$-bonds are omitted. The number of carbon atom vertices will be denoted by N_c, the number of internal carbon vertices bounded by three hexagonal rings by N_{Ic}, and the net number of disconnections (positive values) and/or rings (negative values) among the internal edges (edges bounded by two rings) by $d_s = r - 2 - N_{Ic}$. For example, anthracene/phenanthrene has $d_s = 1$ and $N_{Ic} = 0$ and pyrene has $d_s = 0$ and $N_{Ic} = 2$. A *strictly peri-condensed* benzenoid hydrocarbon has all its internal third degree vertices mutually connected ($d_s = 0, -1, -2, \ldots$) and has no cata-condensed appendages. An *excised internal structure* is the set of connected internal vertices usually associated with a strictly peri-condensed benzenoid which has a formula found at the extreme left-hand boundary of the formula periodic table for benzenoid polycyclic aromatic hydrocarbons (PAH6s). For example, the excised internal structure of pyrene is ethene and of coronene is benzene as shown below by the dotted line. Constant-isomer strictly peri-condensed benzenoids have no proximate bay regions and on a per carbon basis have the fewest number of bay regions and are among the benzenoids with the highest $p\pi$ electronic energy [9, 10]. Table 1 presents a summary of the terminology used herein.



Pyrene (ethene)



Coronene (benezene)

Benzenoid enumeration via their excised internal structures

Strictly peri-condensed benzenoid isomers can be generated by enumeration of their excised internal structures. This method has led to the identification of strictly peri-condensed benzenoid series having a constant number of isomers (Tables 2, 3) [3, 4]. For example, the excised internal structures of pyrene ($C_{16}H_{10}$), coronene ($C_{24}H_{12}$), and ovalene ($C_{32}H_{14}$) are ethene, benzene, and naphthalene, respectively, which have no other isomers composed exclusively of hexagonal rings. By successively circumscribing a carbon-atom perimeter around each of these strictly peri-condensed benzenoids of pyrene, coronene, and ovalene the one-isomer series presented in Table 2 are obtained. Note that each time a benzenoid is circumscribed it must be incremented with six hydrogens. One must clearly distinguish between a base excised structure belonging to a constant-isomer series and the ultimate excised internal structure. A base excised internal structure is the first strictly peri-condensed benzenoid of a constant isomer series. For example, pyrene, coronene, and ovalene are based excised internal structures for the one-isomer series summarized in Table 2, whereas ethene, benzene, and naphthalene are their respective ultimate excised internal structures.

Table 2. Constant isomer series of even strictly peri-condensed benzenoids

Series	Number of isomers	Series	Number of isomers
(C_6H_6)	1		
$C_{24}H_{12}$		$C_{106}H_{26}$	38(19)
$C_{54}H_{18}$		$C_{164}H_{32}$	
$C_{96}H_{24}$		$C_{234}H_{38}$	
:::		:::	
$C_{10}H_8$	1		
$C_{32}H_{14}$		$C_{124}H_{28}$	38(19)
$C_{66}H_{20}$		$C_{186}H_{34}$	
$C_{112}H_{26}$		$C_{260}H_{40}$	
$C_{170}H_{32}$		:::	
:::			
$C_{16}H_{10}$	1	$C_{142}H_{30}$	86(47)
$C_{42}H_{16}$		$C_{208}H_{36}$	
$C_{80}H_{22}$		$C_{286}H_{42}$	
$C_{130}H_{28}$		:::	
:::		$C_{162}H_{32}$	128(71)[b]
$C_{22}H_{12}$	2(1)[a]	$C_{232}H_{38}$	
$C_{52}H_{18}$		$C_{314}H_{44}$	
$C_{94}H_{24}$		:::	
$C_{148}H_{30}$		$C_{184}H_{34}$	128(71)
:::		$C_{256}H_{40}$	
$C_{30}H_{14}$	3(1)	$C_{344}H_{46}$	
$C_{64}H_{20}$		:::	
$C_{110}H_{26}$		$C_{206}H_{36}$	$\underline{428}$[c]
$C_{168}H_{32}$		$C_{284}H_{42}$	
:::		$C_{374}H_{48}$	
$C_{40}H_{16}$	3(1)	:::	
$C_{78}H_{22}$			
$C_{128}H_{28}$		$C_{230}H_{38}$	$\underline{616}$
:::		$C_{312}H_{44}$	
$C_{50}H_{18}$	7(2)	$C_{406}H_{50}$	
$C_{92}H_{24}$		:::	
$C_{146}H_{30}$		$C_{256}H_{40}$	$\underline{616}$
:::		$C_{342}H_{46}$	
$C_{62}H_{20}$	12(4)	$C_{440}H_{52}$	
$C_{108}H_{26}$		:::	
$C_{166}H_{32}$		$C_{282}H_{42}$	$\underline{1265}$
$C_{236}H_{38}$		$C_{372}H_{48}$	
:::		$C_{474}H_{54}$	
$C_{76}H_{22}$	12(4)	:::	
$C_{126}H_{28}$		$C_{310}H_{44}$	$\underline{\sim 1800}$
$C_{188}H_{34}$		$C_{404}H_{50}$	
:::		:::	
$C_{90}H_{24}$	27(12)		
$C_{144}H_{30}$		$C_{340}H_{46}$	$\underline{\sim 1800}$[b]
$C_{120}H_{36}$		$C_{438}H_{52}$	
:::		:::	

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[a] The number of less stable diradical isomers is given in parentheses

[b] Predicted values on induction

[c] Sum of radical and nonradical isomers is underlined

Table 3. Constant isomer series of odd strictly peri-condensed benzenoids

Series	No. of isomers	Series	No. of isomers
$C_{13}H_9$ $C_{37}H_{15}$ $C_{73}H_{21}$ $C_{121}H_{27}$ :::	1	$C_{115}H_{27}$ $C_{175}H_{33}$ $C_{247}H_{39}$ :::	48
$C_{19}H_{11}$ $C_{47}H_{17}$ $C_{87}H_{23}$ $C_{139}H_{29}$ :::	1	$C_{133}H_{29}$ $C_{197}H_{35}$ $C_{273}H_{41}$ :::	74
$C_{27}H_{13}$ $C_{59}H_{19}$ $C_{103}H_{25}$ $C_{159}H_{31}$ :::	1	$C_{153}H_{31}$ $C_{221}H_{37}$ $C_{301}H_{43}$ :::	74
$C_{35}H_{15}$ $C_{71}H_{21}$ $C_{119}H_{27}$ $C_{179}H_{33}$ :::	2	$C_{173}H_{33}$ $C_{245}H_{39}$ $C_{329}H_{45}$ :::	174
$C_{45}H_{17}$ $C_{85}H_{23}$ $C_{137}H_{29}$ $C_{201}H_{35}$ :::	4[a]	$C_{195}H_{35}$ $C_{271}H_{41}$ $C_{359}H_{47}$ :::	258
$C_{57}H_{19}$ $C_{101}H_{25}$ $C_{157}H_{31}$ $C_{225}H_{37}$ :::	4	$C_{219}H_{37}$ $C_{299}H_{43}$ $C_{391}H_{49}$ :::	258
$C_{69}H_{21}$ $C_{117}H_{27}$ $C_{177}H_{33}$ :::	13[b]	$C_{243}H_{39}$ $C_{327}H_{45}$ $C_{423}H_{51}$ :::	550
$C_{83}H_{23}$ $C_{135}H_{29}$ $C_{199}H_{35}$ :::	20[b]	$C_{269}H_{41}$ $C_{357}H_{47}$ $C_{457}H_{53}$ :::	796
$C_{99}H_{25}$ $C_{155}H_{31}$ $C_{223}H_{37}$ :::	20	$C_{297}H_{43}$ $C_{389}H_{49}$ $C_{493}H_{55}$ :::	796[c]

[a] In the previous enumeration, one structure was inadvertently overlooked
[b] These two series were published with undetected misprints
[c] Predicted value based on induction

Pyrene is a strictly peri-condensed benzenoid with an ethene excised internal structure. Since ethene is incapable of having isomers, pyrene has no other benzenoid isomer since it has only one arrangement of its internal third degree vertices. There are three isomers of the formula C_4H_6: (Fig. 1) *s-cis*-1,3-butadiene, *s-trans*-1,3-butadiene, and trimethylenemethane diradical. If an 18-carbon-atom perimeter is circumscribed about each of these C_4H_6 isomers with the

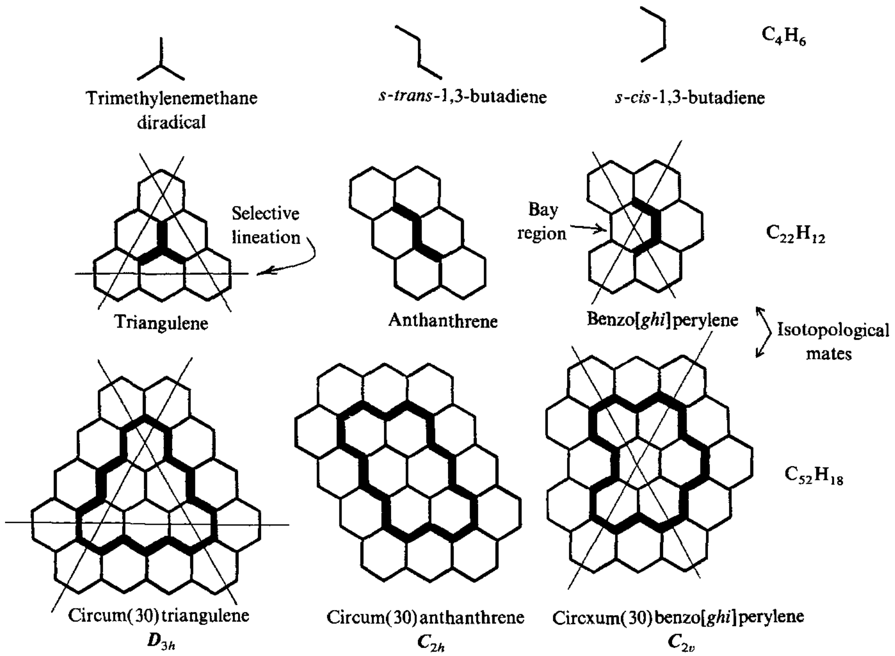
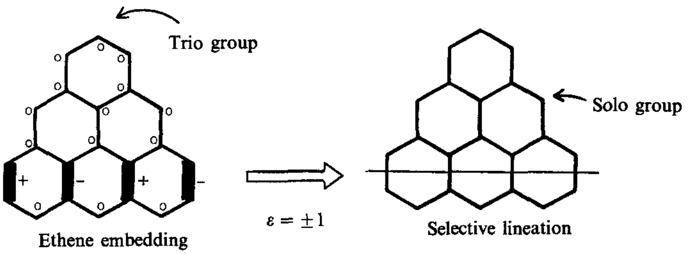


Fig. 1. Illustration of the excised internal structure concept in enumeration of all the benzenoid isomers of $C_{22}H_{12}$, $C_{52}H_{18}$, $C_{94}H_{24}$, . . .

resulting species being incremented with six hydrogens, one obtains the only three $C_{22}H_{12}$ benzenoid isomers possible for this formula, i.e., benzo[*ghi*]perylene, anthanthrene, and triangulene. If these three latter strictly pericondensed benzenoids are circumscribed by a 30-carbon-atom perimeter followed by incrementation with 6 H's, one obtains the only three benzenoid isomers possible for $C_{52}H_{18}$. Because trimethylenemethane is a diradical, triangulene and its $C_{52}H_{18}$ successor are also diradicals (Fig. 1) [4].

That this latter is so can be easily seen by noting that trimethylenemethane diradical (C_4H_6) has one nonstarred and three starred positions, and the 18-carbon-atom annulene ($C_{18}H_{18}$) has an equal number of starred and nonstarred positions. Union of these two structures in such a way as to form triangulene ($C_{22}H_{12}$) by breaking off six hydrogens from each and connecting the carbons leads to an excess of two starred positions. Similarly, repeating this process with triangulene and the 30-carbon-atom annulene again leads to an excess of two starred positions in the $C_{52}H_{18}$ successor benzenoid. Thus, no Kekule' structure having an edge joining every starred position once to an adjacent nonstarred position can be drawn for these structures, and they all will possess two nonbonding MOs.

Whenever a benzenoid structure can have a succession of parallel edges bisected with a straight line drawn from one side of the molecule to the other with the terminal rings being symmetrically convex relative to the line, then those edges intersected can be embedded with a succession of ethene substructures and the benzenoid structure as a whole will have at least one eigenvalue pair of plus and minus one (for the graph's adjacency matrix) [9]. A selective lineation is a maximal orthogonal secant passing through a benzenoid structure such that the bisected terminal edges are central to a duo, trio, or quartet perimeter subsection. This definition is illustrated with triangulene below.



Constant-isomer series of strictly peri-condensed benzenoids

Tables 2 and 3 present all known benzenoid constant-isomer series in which the latter are now reported for the first time [4]. Each table reveals the same distinct pattern in which the number of isomers alternate between singlet and doublet occurrence. Also, the pattern for the progressive increase in the first member formula of each series should be evident and will allow one to extend these tables even further. As it will now be shown each pair of series with the same isomer number possess a one-to-one correspondence of the following topological parameters between their benzenoid members. There are three topological parameters considered: Symmetry and the number of bay regions and selective lineations possessed by the benzenoid. When two benzenoids are identical in these parameters, they are said to be isotopological. These three parameters have been identified as having a one-to-one mapping between appropriate benzenoid pairs where one benzenoid may be selected from each of the two constant-isomer series with the same isomer number or within a single constant-isomer series. These parameters are topological invariants. Within a constant-isomer series the benzenoid members have isotopological mates in going from one isomer set to another. See Fig. 1 for an example of a constant-isomer series with a bay region, selective lineations, and isotopological mates.

Topological characteristics

The one-isomer series (Table 2) beginning with benzene is unique (belongs to the singlet occurrence isomer class) and has corresponding benzenoids with D_{6h} symmetry. Both the other two one-isomer series starting with naphthalene and pyrene have benzenoids with D_{2h} symmetry and one selective lineation. The constant-isomer series starting with $C_{22}H_{12}$ is unique. Both the constant-isomer series starting with $C_{30}H_{14}$ and $C_{40}H_{16}$ have benzenoids that are pairwise equivalent. Even-carbon strictly peri-condensed benzenoids up to $C_{46}H_{18}$ can only possess nonradical and diradical isomers. Both the diradicals, dibenzo[*bc,hi*]coronene ($C_{30}H_{14}$) and phenalenyl[2,3,4,5-*hijk*]ovalene ($C_{40}H_{16}$), have C_{2v} symmetry, no bay regions, and one selective lineation [7]. Naphtho[1,8,7-*abc*]coronene ($C_{30}H_{14}$) and anthra[2,1,9,8-*hijkl*]ovalene ($C_{40}H_{16}$) both have C_s symmetry, one bay region, and two selective lineations. Dibenzo[*bc,ef*]coronene ($C_{30}H_{14}$) and phenanthro[3,4,5,6-*efghi*]ovalene ($C_{40}H_{16}$) both have C_{2v} symmetry, one bay region, and no selective lineation. Finally, dibenzo[*bc,kl*]coronene and circumanthracene both have D_{2h} symmetry, no bay region, and one selective lineation [7]. Figures 2 to 5 give all the benzenoids of the constant-isomer series starting with $C_{62}H_{20}$ and $C_{76}H_{22}$, and it can be verified that each group has a one-to-one correspondence in regard to their symmetry, bay regions, and selective lineations.

The one-isomer series (Table 3) beginning with phenalenyl ($C_{13}H_9$) is unique and has benzenoids with D_{3h} symmetry. The one-isomer series starting with $C_{19}H_{11}$ and $C_{27}H_{13}$ have benzenoids with C_{2v} symmetry, no bay regions, and one selective linearation. The constant-isomer series starting with $C_{45}H_{17}$ and $C_{57}H_{19}$ are shown in Figs. 6 and 7, respectively, and form topologically equivalent benzenoid groups. The constant-isomer series starting with $C_{83}H_{23}$ and $C_{99}H_{25}$ both have $16C_s$ and $4C_{2v}$ benzenoids. These two strictly peri-condensed benzenoids can only possess mono- and triradical isomers, the relative number of which is the same. Note that no odd carbon monoradical or even-carbon diradical strictly peri-condensed benzenoid can have C_{2h} and D_{2h} symmetry. Thus, the constant-isomer series with the same isomer number possess and isotopological equivalence between their benzenoid members (Table 4).

For the constant-isomer series in Tables 2 to 4, the diradical benzenoids (Table 2) have a one-to-one correspondence to the monoradical benzenoids (Table 3). The $C_{22}H_{12}$ diradical (triangulene) and $C_{13}H_9$ monoradical (phenalenyl) both the D_{3h} symmetry, no bay regions, and three selective lineations. The $C_{30}H_{14}$ diradical and $C_{19}H_{11}$ monoradical both have C_{2v} symmetry, no bay regions, and one selective lineation as do the $C_{40}H_{16}$ diradical and the $C_{27}H_{13}$ monoradical. The two $C_{50}H_{18}$ diradicals and the two $C_{35}H_{15}$ monoradicals all have C_s symmetry and a member of each pair has one bay region and two selective lineations while the other has neither. There is a one-to-one correspondence between the four diradicals of $C_{62}H_{20}$ and the four monoradicals of $C_{45}H_{17}$ as there is for the four diradicals of $C_{76}H_{22}$ and the four monoradicals of $C_{57}H_{19}$ (Figs. 4–7). There is a one-to-one correspondence between the 12 diradicals of $C_{90}H_{24}$ and 12 of monoradicals of $C_{69}H_{21}$ (Figs. 8, 9). In addition, $C_{69}H_{21}$ possesses a triradical shown as the last structure in Fig. 9. In regard to symmetry, number of bay regions, and number of selective lineations there is again a one-to-one correspondence between that 19 ($16C_s + 3C_{2v}$) $C_{106}H_{26}$ and $C_{124}H_{28}$ benzenoid diradicals and the 19 $C_{83}H_{23}$ and $C_{99}H_{25}$ benzenoid monoradicals. The additional triradical benzenoid isomers of $C_{83}H_{23}$ and $C_{99}H_{25}$ are shown in Fig. 10.

Table 4. Parameters of benzenoid members of various pairwise equivalent constant-isomer series

Series, initial	Symmetry group (number zero and ± 1 eigenvalues) numbered PAH6s[a]			
formula	$n_0 = 0$[b]	$n_0 = 1$	$n_0 = 2$	$n_0 = 3$
$C_{30}H_{14}$ $C_{40}H_{16}$	$C_{2v}(0^2, 1) - 1, D_{2h}(1) - 1$	$C_s(1^2) - 1, C_{2v} - 1$		
$C_{62}H_{20}$ $C_{76}H_{22}$	$C_{2h} - 1, C_{2v}(0^2, 1) - 1$	$C_s - 1, C_s(0^2) - 1, C_s(1) - 2,$ $C_s(1^2) - 1, C_s(0^2, 1^2) - 2,$ $C_{2v} - 1$	$C_s(1) - 2, C_{2h}(1) - 1,$ $C_{2v}(1^3) - 2, D_{2h}(1^2) - 1$	
$C_{106}H_{26}$ $C_{124}H_{28}$	$C_s(0^2) - 1$	$C_s - 4, C_s(0^2) - 3, C_s(1) - 3,$ $C_s(1^2) - 2, C_s(0^2, 1) - 4,$ $C_s(0^2, 1^2) - 2$	$C_s - 4, C_s(1) - 9, C_s(1^2) - 3,$ $C_s(1^3) - 2, C_{2h}(1^2) - 1,$ $C_{2v}(1) - 3, C_{2v}(1^2) - 1,$ $C_{2v}(0^2, 1^2) - 1, C_{2v}(0^2, 1^3) - 2,$ $C_s(0^2, 1) - 5, C_s(0^2, 1^3) - 1$	$C_s - 1, C_s(1^2) - 2,$ $C_s(1^3) - 1, C_{2v}(1^2) - 2$
$C_{45}H_{17}$ $C_{57}H_{19}$	$C_{2v}(0, 1) - 1$	$C_s(0) - 1, C_s(0, 1^2) - 2$		
$C_{83}H_{23}$ $C_{99}H_{25}$	$C_s(0) - 1, C_{2v}(0^3) - 1$	$C_s(0) - 3, C_s(0, 1) - 4,$ $C_s(0, 1^2) - 2$	$C_s(0, 1) - 5, C_s(0, 1^3) - 1,$ $C_{2v}(0, 1^2) - 1, C_{2v}(0, 1^3) - 2$	

[a] $C_{2v}(0^2, 1^3) - 2$ means that in each relevant series there are 2 benzenoids of C_{2v} symmetry and the same number of bay regions (n_0) with 2 zero eigenvalues (diradicals) and 3 selective lineations (3 eigenvalue pairs of ± 1)

[b] In columns with the same number of bay regions (n_0)

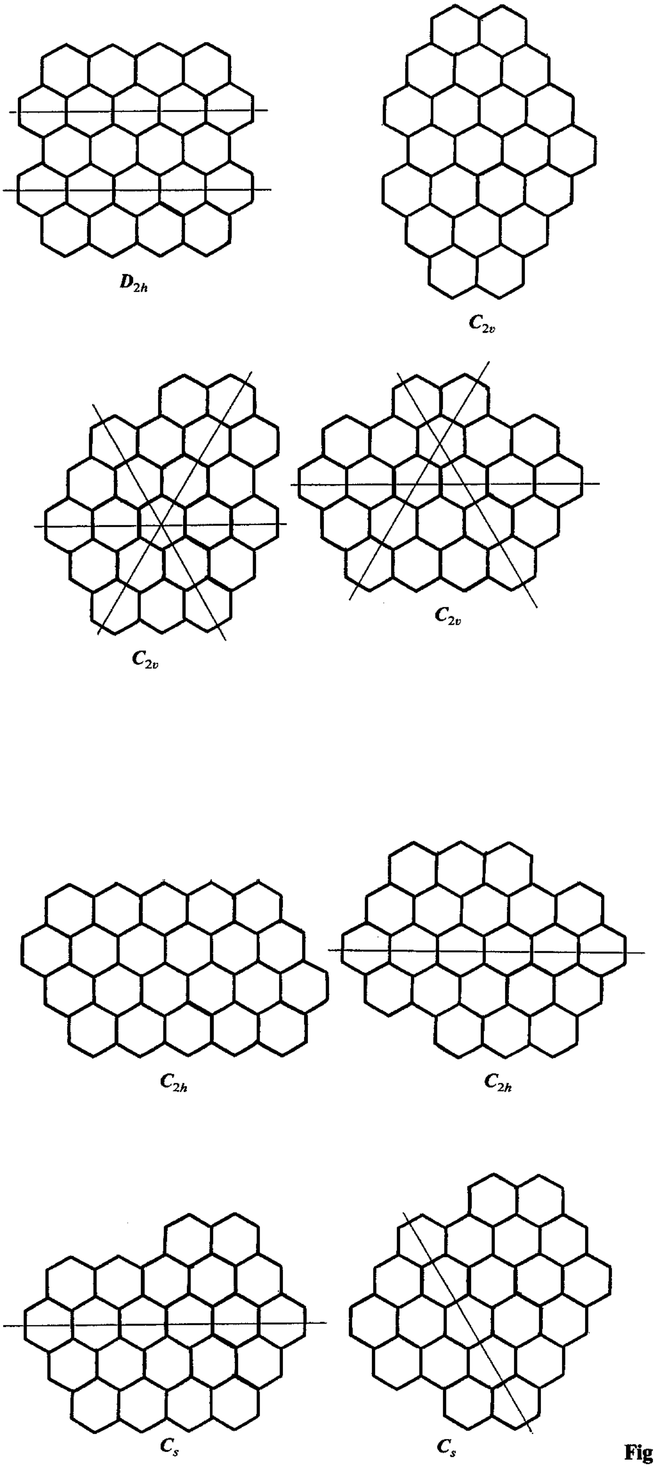


Fig. 2

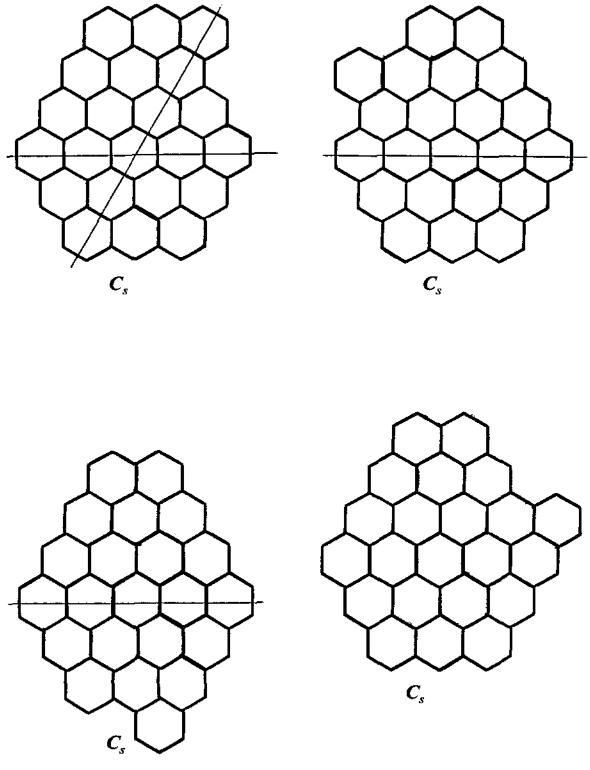
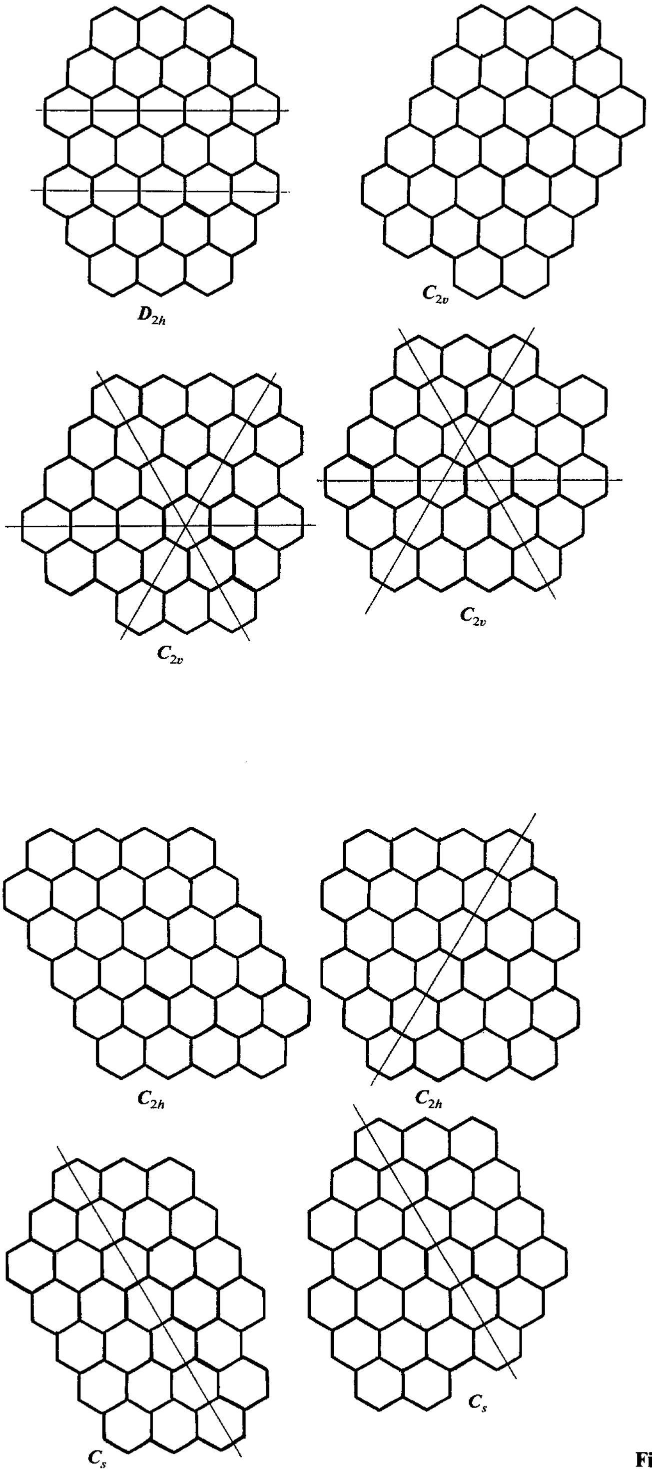


Fig. 2. Base members of the $C_{62}H_{20}$ constant-isomer benzenoid series

From the results in the prior paragraph, if this one-to-one correspondence of even-carbon diradicals and odd-carbon monoradicals continues, then all one needs to do is deduce the number of even-carbon tetraradicals in the $C_{142}H_{30}$ constant-isomer series and the number of odd-carbon triradicals in the $C_{115}H_{27}$ constant-isomer series and substract the difference from 48 to determine number of radical isomers in the $C_{142}H_{30}$ constant-isomer series. In doing this, one tetraradical and two triradicals were found for which the ultimate excised internal structures are given in Fig. 11. Thus, we predicted and verified that there are 86 nonradical and 47 radical benzenoids for the $C_{142}H_{30}$ constant-isomer series. Similarly, one tetraradical for $C_{162}H_{32}$ and $C_{184}H_{34}$ each and four triradicals for $C_{133}H_{29}$ and $C_{153}H_{31}$ each were found for which the ultimate excised internal structures are given in Fig. 12. Thus, 128 nonradical and 71 radical isomers were predicted and verified for both the constant-isomer series beginning with $C_{162}H_{32}$ and $C_{184}H_{34}$. It is important to note that triradicals do not enter until $C_{69}H_{21}$ which has one isomer with a penultimate (next to the last) excised internal structure of tetraangulene ($C_{33}H_{15}$) which is a triradical. Similarly, tetraradicals did not enter until $C_{142}H_{30}$ which has one isomer with a penultimate excised internal structure of pentaangulene ($C_{46}H_{18}$). By analogy one should not expect pentaradicals or hexaradicals to enter until $C_{325}H_{45}$ (hexaangulene penultimate excised internal structure of $C_{61}H_{21}$) and $C_{706}H_{66}$ (heptaangulene penultimate excised internal structure of $C_{78}H_{24}$), respectively. The origin of the



D_{2h} C_{2v}

C_{2v} C_{2v}

C_{2h} C_{2h}

C_s C_s

Fig. 3

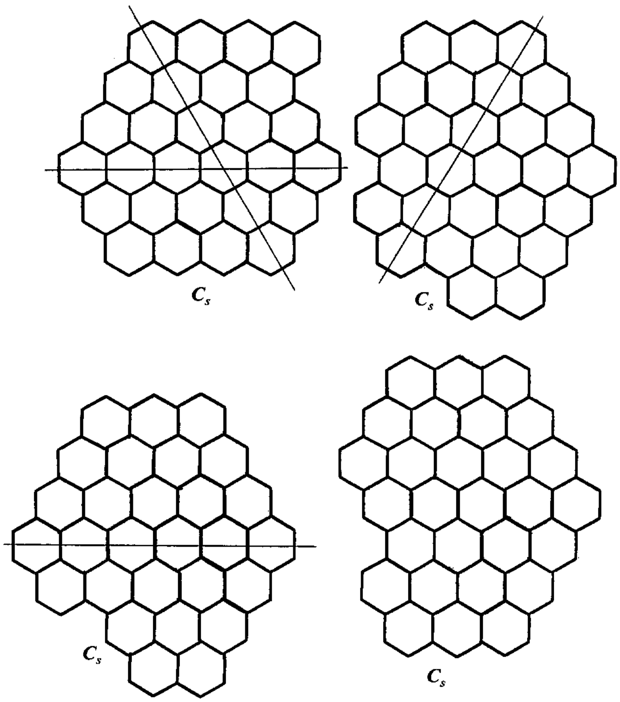


Fig. 3. Base members of the $C_{76}H_{22}$ constant-isomer benzenoid series

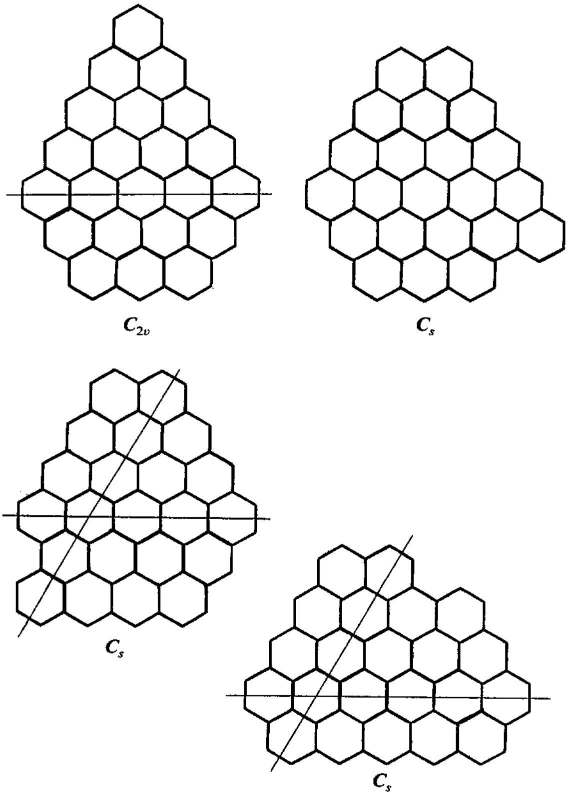


Fig. 4. Diradical base members of the $C_{62}H_{20}$ constant-isomer benzenoid series

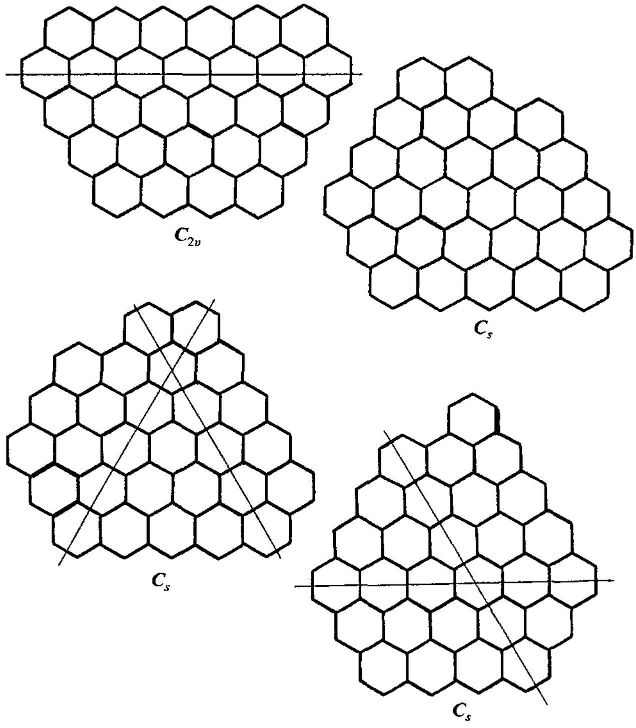


Fig. 5. Diradical base members of the $C_{76}H_{22}$ constant-isomer benzenoid series

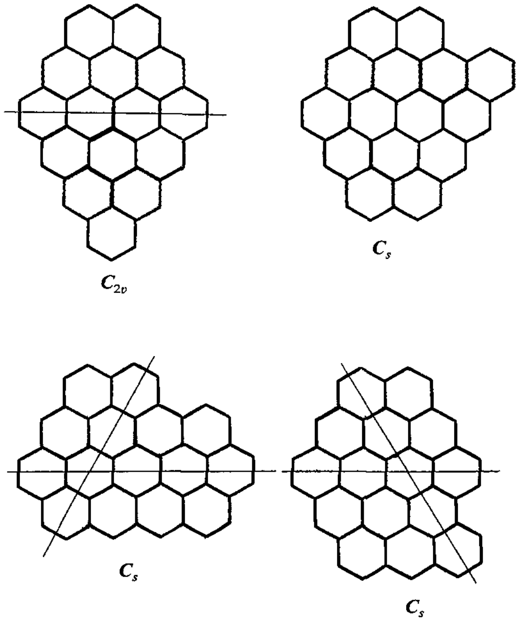


Fig. 6. Base members of the $C_{45}H_{17}$ constant-isomer benzenoid series

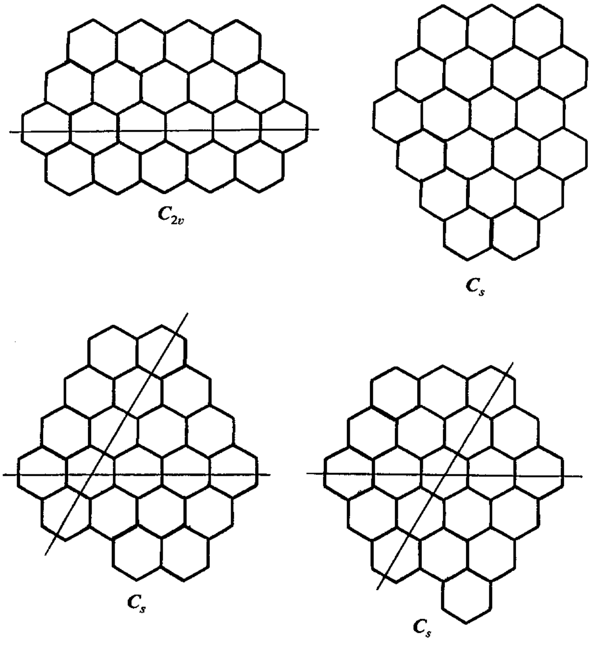


Fig. 7. Base members of the $C_{57}H_{19}$ constant-isomer benzenoid series

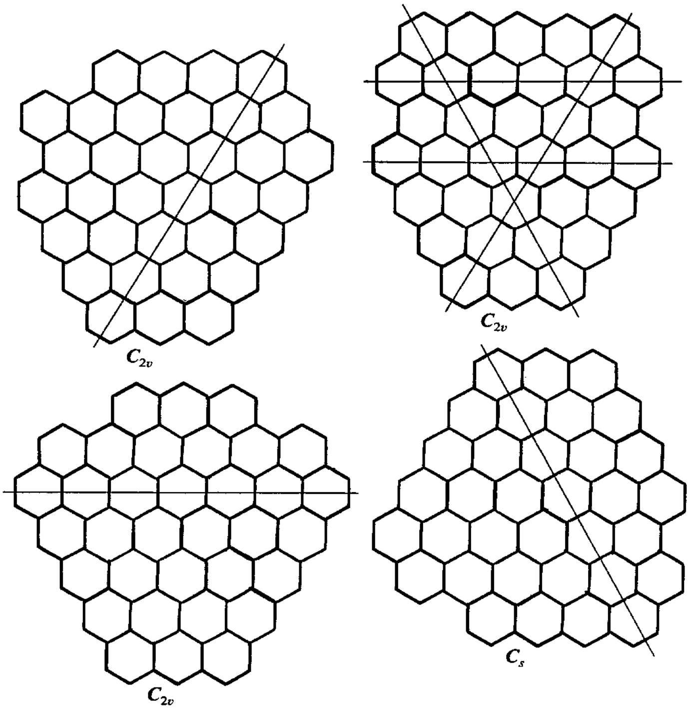
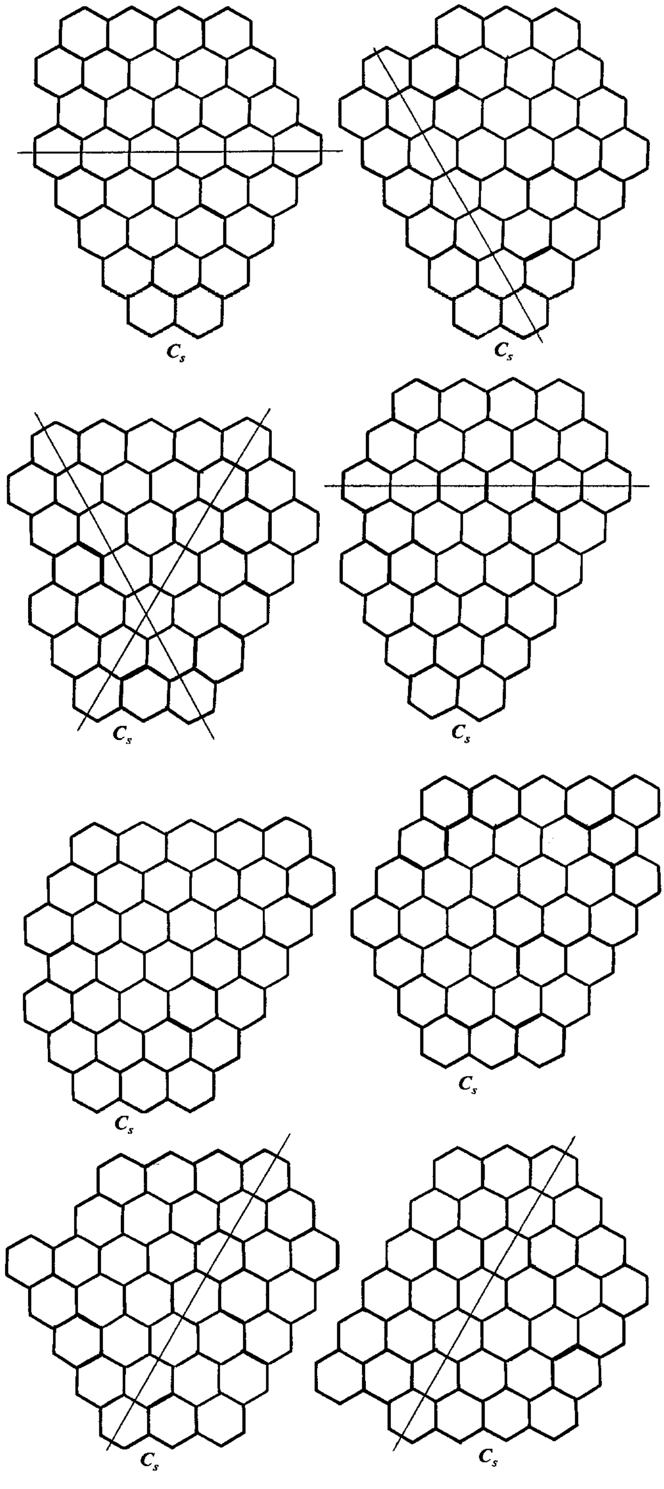


Fig. 8



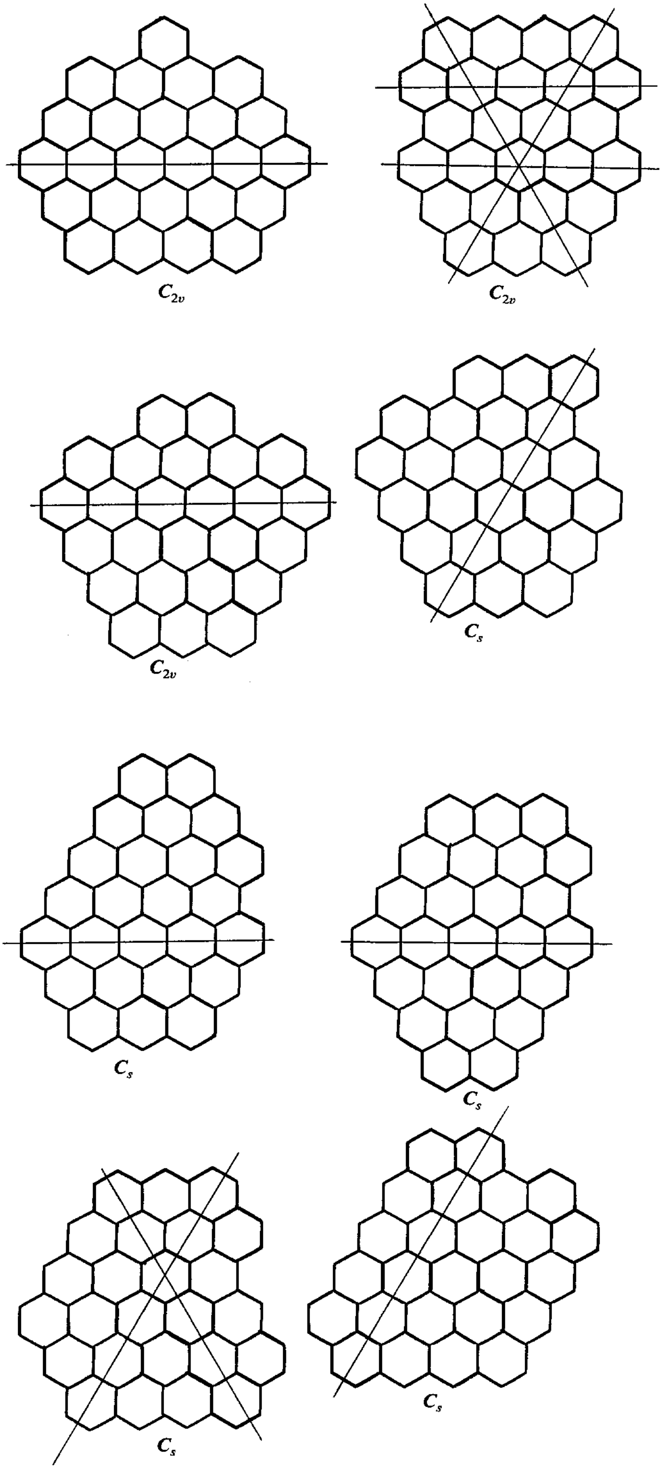
C_s C_s

C_s C_s

C_s C_s

C_s C_s

Fig. 8. The 12 diradical benzenoids of $C_{90}H_{24}$



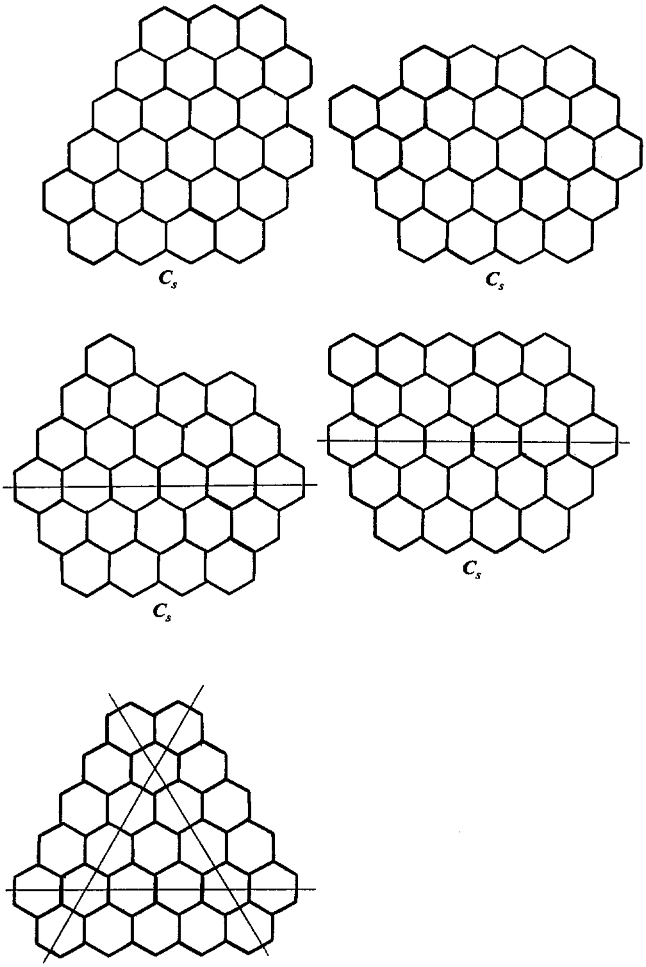
C_{2v} C_{2v}

C_{2v} C_s

C_s C_s

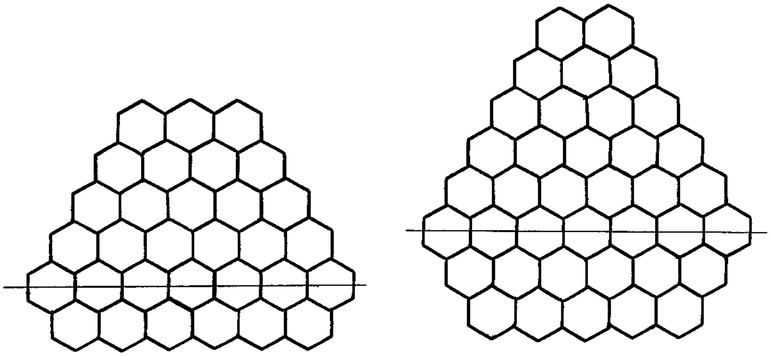
C_s C_s

Fig. 9



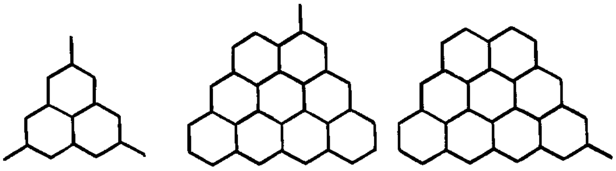
C_s C_s C_s C_s D_{3h}

Fig. 9. The 13 radical benzenoids of $C_{69}H_{21}$



$C_{83}H_{23}$, C_{2v} $C_{99}H_{25}$, C_{2v}

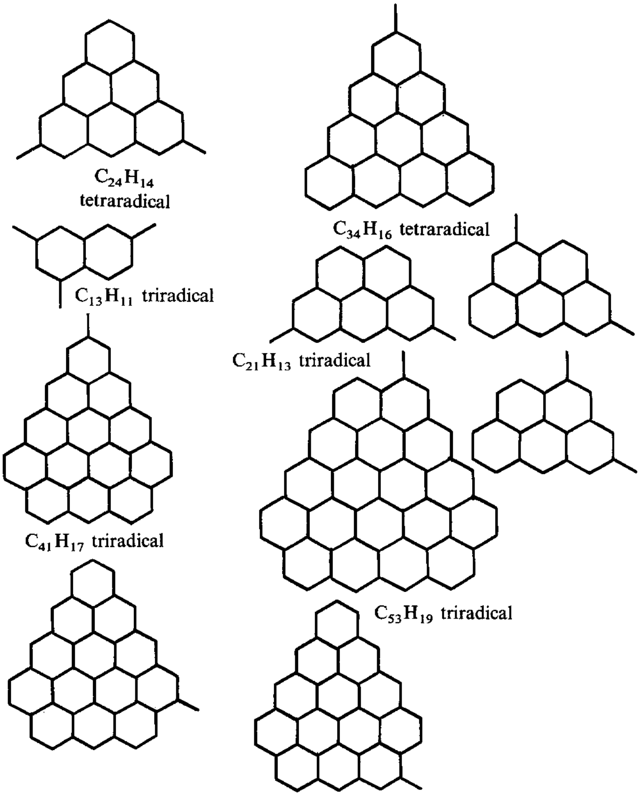
Fig. 10. The triradical benzenoids of $C_{83}H_{23}$ and $C_{99}H_{25}$



$C_{16}H_{12}$
tetraradical

$C_{31}H_{15}$
triradicals

Fig. 11. Excised internal structures of the constant-isomer series beginning with $C_{142}H_{30}$ and $C_{115}H_{27}$, respectively



$C_{24}H_{14}$
tetraradical

$C_{34}H_{16}$ tetraradical

$C_{13}H_{11}$ triradical

$C_{21}H_{13}$ triradical

$C_{41}H_{17}$ triradical

$C_{53}H_{19}$ triradical

Fig. 12. Excised internal structures of the constant-isomer series beginning with $C_{162}H_{32}$, $C_{184}H_{34}$, $C_{133}H_{29}$, and $C_{153}H_{31}$

isotopological equivalence between certain odd-carbon monoradical and even-carbon diradical benzenoids belonging to the constant-isomer series arises from the common threefold symmetry of the centralized methyl radical and trimethylenemethane diradical substructures in a polyhex system.

Summary

Tables 2 and 3 greatly extend the isomer numbers found in previous work of benzenoid hydrocarbons [8, 11]. As it has been herein demonstrated these strictly peri-condensed benzenoids having formulae along the left-hand staircase boundary of Table PAH6 have unique characteristics and form alternating pairs of topologically equivalent sets of benzenoid structures with the nonidentical invariants of N_c, N_{Ic}, q, and r. This work again demonstrates the power of Table PAH6 to sort benzenoid formulas into a hierarchal order forming series with unique characteristics. Of particular significance are the strictly peri-condensed benzenoid structures located on the left-hand staircase edge of Table PAH6. These benzenoids have topologies that are intricately related to what we call an edge effect of Table PAH6. This edge effect appears to be governed by a fundamental topological principle which limits the number of possible arrangements of hexagons. Specifically, we have more fully defined the prerequisite properties of a periodic table set, have identified an edge effect phenomenon, and have characterized a topological relationship within a benzenoid constant-isomer series and between two related constant-isomer series.

Since constant-isomer benzenoids cannot have helicenic or circulene forms, their isomer numbers are totally unambiguous. Strictly peri-condensed benzenoids are fundamentally planar systems that are incapable of exhibiting stereoisomers. These strictly peri-condensed benzenoids are believed to be ultimate carbonization/pyrolytic constituents.

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