

A FORMULA PERIODIC TABLE FOR BENZENOID HYDROCARBONS AND THE AUFBAU AND EXCISED INTERNAL STRUCTURE CONCEPTS IN BENZENOID ENUMERATIONS

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Abstract

The genesis of the aufbau and excised internal structure concepts is traced. These concepts were pivotal to the first published enumerations of the strictly peri-condensed, non-Kekuléan, and essentially strain-free total resonant sextet benzenoid groups. A *periodic table set* is defined as a partially ordered set 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.

1. Introduction

Our 1978–1980 work dealing with the priority pollutants under the aegis of the Environmental Protection Agency, Region VII [1–3], made it evident that benzenoid hydrocarbons were ubiquitous pyrolytic pollutants which needed systematic study. When I subsequently went on a Fulbright Senior Lectureship to the University of Ljubljana, Yugoslavia during the Winter Semester of 1981, I had the opportunity to delve into the problem of analyzing the formula/isomer relationships of benzenoid hydrocarbons. It seemed to me that a reasonable relationship must exist. At the time, I was only aware of Eric Clar's two-volume work [4] and Balaban and Harary's Tetrahedron paper [5]. This latter paper dealt exclusively with enumeration of cata-condensed benzenoid hydrocarbons. Several events converged at this time. First, I developed my formula table and aufbau and excised internal structure concepts in rudimentary form. Second, I was invited by Professor Trinajstić to present a lecture on these results [6] and for a return visit to lecture on the priority pollutants. It was Professor Trinajstić who named my formula table "a periodic table". This work was the first to emphasize enumeration of peri-condensed benzenoid hydrocarbons [7].

Our work has always been concerned with enumeration of chemically relevant benzenoid compounds rather than wholesale enumeration of polyhexes [8]. The first publication of the excised internal structure concept was associated with the first enumeration of strictly peri-condensed benzenoid isomers, which are predicted to be among the ultimate pyrolytic products [9]. The first reported work dealing with the *exclusive* enumeration of non-Kekuléan benzenoids was stimulated by their presumed intermediacy in combustion processes [10]. A master structure and corresponding

method for enumerating total resonant sextet benzenoids was proposed in the seminal paper [11] which inspired the subsequent work of Knop and coworkers [12]. This led to the first enumeration of essentially strain-free total resonant sextets of potential interest to analytical/environmental scientists [13,14].

2. A formula periodic table for benzenoid hydrocarbons

The formulas for all benzenoids are found in table 1, which has x, y -coordinates of (d_s, N_{Ic}) . Recursive construction of this table was accomplished using the aufbau principle (*vide infra*). Table 1 complies with a sextet rule analogous to the octet rule for the periodic table of elements, and d_s is analogous to the outer-shell electronic configuration and N_{Ic} is analogous to the principal quantum number associated with the periodic table of elements. Thus, table 1 can be described as being "Mendeleevian" [15]. The terminology used herein is summarized in the appendix.

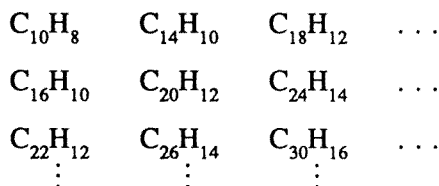
Table 1 represents a partially ordered set which sorts benzenoid hydrocarbons into isomer groups and identifies their group properties [16,17]. The graph-theoretical invariants (GI) that remain unchanged among polyhex isomers are known:

$$GI(\text{PAH6}) = \{a_4, a_6 + n_0, a_8^c, d_s, N_{Ic}, N_c, N_H, q, q_1, r\}.$$

These absolute group properties are fixed and are useful in studying differences among isomer groups. For example, the average HMO electronic $p\pi$ energy between isomer groups is principally determined by N_c and q . To study differences among PAH6 isomers, one needs graphical invariants that change from one isomer to another. No unique and simple invariant for all PAH6 isomers has yet been identified. Computed HMO eigenvalues appear to be unique but are not simply obtained through inspection. If the simplicity requirement could be fulfilled, this would facilitate our conceptualization and thinking processes about these systems. In the meantime, we must be satisfied with HMO eigenvalues for discerning among PAH6 isomers. If one is interested in a subset of PAH6 structures that are somehow related, as a homologous series, then the hierarchical relationships among the nonisomeric homologous members are prescribed by table 1.

In 1829, Johann Wolfgang Dobereiner noted that certain similar elements occurred in groups of three, which he called triads. The atomic weight of the middle member of a triad is very nearly equal to the arithmetic mean of the atomic weights of the other two members of the triad. For instance, the triad of chlorine (at. wt. = 35.5), bromine (at. wt. = 79.9) and iodine (at. wt. = 126.9) gives $(35.5 + 126.9)/2 = 81.2$ for the atomic weight mean of Cl and I, which can be compared with 79.9 for Br. It is now known that the atomic number of the middle member of a triad is exactly equal to the arithmetic mean of the atomic numbers of the other two element members of the triad. For instance, the triad of chlorine (atomic number = 17), bromine (atomic number = 35) and iodine (atomic number = 53) gives $(17 + 53)/2 = 35$ for the atomic number mean of Cl and I, which can be compared with 35 for Br. The formula periodic table for

benzenoid hydrocarbons (table 1) follows Dobereiner's triad principle. Consider the following small section of table 1:



Whether one goes horizontally along a row, vertically in a column, or diagonally, the middle formula of a triad is always the arithmetic mean of the other two.

The criteria for a *periodic table set* are that it is a partially ordered set (obeys reflexivity, antisymmetry, and transitivity) forming a two-dimensional array which complies with Dobereiner's *triad principle*, where the middle member (element) has a metric property that is the arithmetic mean of the other two surrounding adjacent members. Both the periodic table of elements and table 1 are sets that embody these attributes, which constitute a formal definition of a periodic table set.

3. HMO $p\pi$ electron energy and eigenvalue correlations

Through a vector addition analog method, we previously showed that the total $p\pi$ energy (E_π^L) of a large benzenoid hydrocarbon can be estimated from the known E_π^L values of smaller ones [10]. Thus, when the number of carbon (N_c^L) and hydrogen (N_H^L) atoms of a large benzenoid hydrocarbon is related by $(N_c^L, N_H^L) = (N_c, N_H) + (N'_c, N'_H) = (N_c + N'_c, N_H + N'_H)$ to the number of carbon and hydrogen atoms of smaller benzenoid hydrocarbons, then $E_\pi^L = E_\pi + E'_\pi$. Since both $N_c^L = N_c + N'_c$ and $q^L = q + q'$ are overall conserved quantities, the level accuracy of the vector predicted E_π^L is better than the approximations due to McClelland [18] ($E_\pi \leq \sqrt{2qN_c}$) or Hall [19] ($E_\pi = q + \frac{1}{3}N_c$) because of the input of known E_π and E'_π values for the smaller benzenoids. For example, in the vector addition of $(10, 8) + (28, 14) = (38, 22)$ naphthalene ($E_\pi = 13.68\beta$) plus a $\text{C}_{28}\text{H}_{14}$ isomer ($E'_\pi = 40.08 - 40.37\beta$) would go to a $\text{C}_{38}\text{H}_{22}$ PAH6 isomer ($E_\pi^L = 53.26 - 54.06\beta$), giving a better E_π^L estimate (54.1β) than $E_\pi^L = \sqrt{2 \cdot 46 \cdot 38}\beta = 59.13\beta$ or $E_\pi^L = (46 + \frac{1}{3} \cdot 38)\beta = 58.67\beta$ due to McClelland or Hall, respectively.

Recently, Cioslowski published a new and more precise upper bound for E_π . Using his graph topological equation for the above example, one obtains $E_\pi = 58.01\beta$, which can be compared to the actual value of $E_\pi = 54.06\beta$. Although his value is better than that obtained by Hall's equation, it is still inferior to our method. Our method does have its limitation, since not all benzenoid formulas are accessible via the vector addition described above.

$N_c = 3N_H - 16$	$N_c = 3N_H - 18$	$N_c = 3N_H - 20$	$N_c = 3N_H - 22$	$N_c = 3N_H - 24$	$N_c = 3N_H - 26$	$N_c = 3N_H - 28$	$N_c = 3N_H - 30$	$N_c = 3N_H - 32$	$N_c = 3N_H - 34$
$C_{14}H_{10}$	$C_{18}H_{12}$	$C_{22}H_{14}$	$C_{26}H_{16}$	$C_{30}H_{18}$	$C_{34}H_{20}$	$C_{38}H_{22}$	$C_{42}H_{24}$	$C_{46}H_{26}$	$C_{50}H_{28}$
$C_{20}H_{12}$	$C_{24}H_{14}$	$C_{28}H_{16}$	$C_{32}H_{18}$	$C_{36}H_{20}$	$C_{40}H_{22}$	$C_{44}H_{24}$	$C_{48}H_{26}$	$C_{52}H_{28}$	$C_{56}H_{30}$
$C_{26}H_{14}$	$C_{30}H_{16}$	$C_{34}H_{18}$	$C_{38}H_{20}$	$C_{42}H_{22}$	$C_{46}H_{24}$	$C_{50}H_{26}$	$C_{54}H_{28}$	$C_{58}H_{30}$	$C_{62}H_{32}$
$C_{32}H_{16}$	$C_{36}H_{18}$	$C_{40}H_{20}$	$C_{44}H_{22}$	$C_{48}H_{24}$	$C_{52}H_{26}$	$C_{56}H_{28}$	$C_{60}H_{30}$	$C_{64}H_{32}$	$C_{68}H_{34}$
$C_{38}H_{18}$	$C_{42}H_{20}$	$C_{46}H_{22}$	$C_{50}H_{24}$	$C_{54}H_{26}$	$C_{58}H_{28}$	$C_{62}H_{30}$	$C_{66}H_{32}$
$C_{44}H_{20}$	$C_{48}H_{22}$	$C_{52}H_{24}$	$C_{56}H_{26}$	$C_{60}H_{28}$	$C_{64}H_{30}$
$C_{50}H_{22}$	$C_{54}H_{24}$	$C_{58}H_{26}$	$C_{62}H_{28}$	$C_{66}H_{30}$
$C_{56}H_{24}$	$C_{60}H_{26}$	$C_{64}H_{28}$	$C_{68}H_{30}$
$C_{62}H_{26}$	$C_{66}H_{28}$
$C_{68}H_{28}$

$$2 < N_c/N_H < 3$$

$N_c = 3N_H - 36$	$N_c = 3N_H - 38$	$N_c = 3N_H - 40$	$N_c = 3N_H - 42$	$N_c = 3N_H - 44$...	$(N_c = 2N_H - 6 + N_{1c})$
$C_{54}H_{30}$	$C_{58}H_{32}$	$C_{62}H_{34}$	$C_{66}H_{36}$	$C_{70}H_{38}$...	$N_c = 2N_H - 6$
$C_{60}H_{32}$	$C_{64}H_{34}$	$C_{68}H_{36}$	$C_{72}H_{38}$	$N_c = 2N_H - 4$
$C_{66}H_{34}$	$N_c = 2N_H - 2$
$C_{72}H_{36}$	$N_c = 2N_H$
...	$N_c = 2N_H + 2$
...	$N_c = 2N_H + 4$
...	$N_c = 2N_H + 6$
...	$N_c = 2N_H + 8$
...	$N_c = 2N_H + 10$
...

Since no vector sum corresponds to a strictly peri-condensed benzenoid having a formula on the extreme staircase-like edge of table 1, these benzenoid species cannot have their E_π estimated by this method. One should note the numerous papers written by Gutman on this subject alone [21]. As a final example of our vector addition method for estimating E_π of large benzenoid hydrocarbons, consider isoviolanthrene ($C_{34}H_{18}$), which has $E_\pi = 48.5320\beta$. Vector addition of $(2, 4) + (32, 14) = (34, 18)$ using ethene ($E_\pi = 2.0\beta$) and ovalene ($E_\pi = 46.4974\beta$) gives $E_\pi = 48.4974\beta$ as an estimate for the electronic $p\pi$ energy of isoviolanthrene. Cioslowsky's nodal increment method gives $E_\pi = 48.6616\beta$ for isoviolanthrene [22].

The presence and minimum degeneracy of eigenvalues of $\varepsilon = 0$ and ± 1.0 can be rapidly determined by the following topological rules [17].

Rule 1

If the adjacency matrix of the excised internal structure has an eigenvalue of zero, then the adjacency matrix of the corresponding non-perylene-like strictly peri-condensed benzenoid structure also has an eigenvalue of zero.

Phenalenyl monoradical ($C_{13}H_9$) is a strictly peri-condensed PAH6 with the methyl radical as an excised internal structure, and both have adjacency matrices with $\varepsilon = 0$. The diradical $C_{22}H_{12}$ isomer, triangulene, is a strictly peri-condensed benzenoid hydrocarbon and has the trimethylenemethane diradical as an excised internal structure; both triangulene and trimethylenemethane diradicals have adjacency matrices with two eigenvalues of $\varepsilon = 0$. Perylene-like molecules, such as dibenzo[*fg, op*]-anthanthrene, have cross-conjugated diradical excised internal structures and represent exceptions to this rule.

Rule 2

Whenever a benzenoid structure can have a succession of 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 rings intersected by the line can be embedded with a perpendicular succession of ethene substructures, and the benzenoid structure as a whole will have an adjacency matrix with at least one eigenvalue pair of plus and minus one. This straight line will be called a selective lineation (fig. 1).

If a parent benzenoid excised internal structure has one or more selective lineations, then the larger daughter benzenoid structure will also have an identical number of selective lineations. For each distinct selective lineation present in an alternant hydrocarbon there will be a corresponding eigenvalue pair of $\varepsilon = \pm 1.0\beta$. Thus, coronene has three selective lineations and is triply degenerate in $\varepsilon = \pm 1.0\beta$, and perylene has four selective lineations and is quadruply degenerate in $\varepsilon = \pm 1.0\beta$. Benzene has three distinct ethene embeddings, but only two of them are mutually exclusive.

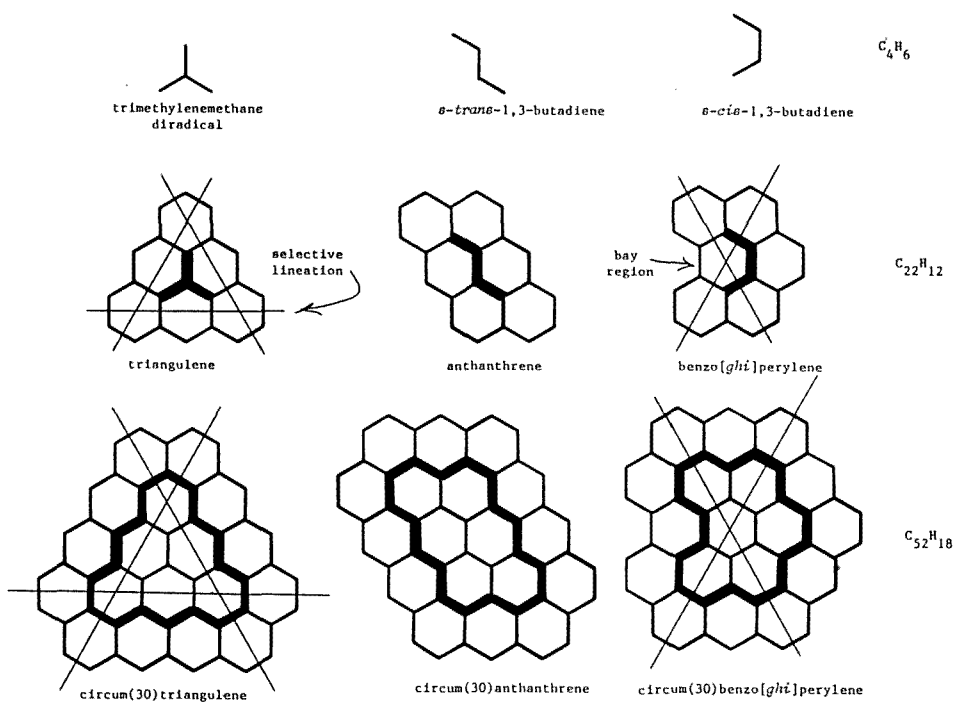
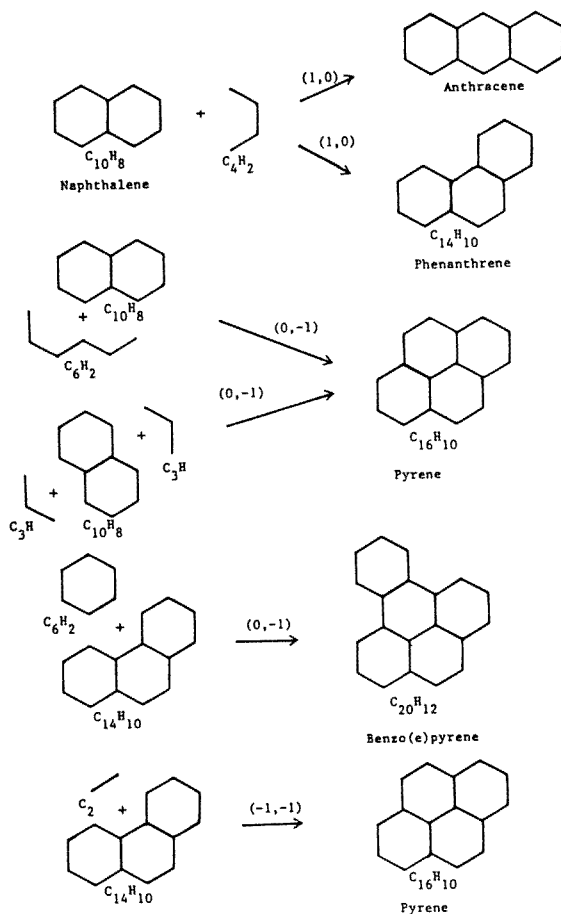


Fig. 1. Illustration of the excised internal structure concept in the enumeration of all the benzenoid isomers of $C_{22}H_{12}$, $C_{52}H_{18}$, $C_{94}H_{24}$, etc.

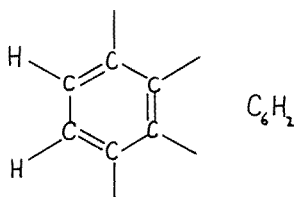
4. The aufbau principle

The aufbau principle was anticipated by Clar's annellation method for correlating UV absorption spectral trends for various series of benzenoid compounds in which the number of bay regions and resonant sextets were generally held fixed [2]. In 1981, two postulates were stated [7]. First, the formula for any benzenoid hydrocarbon is found in our formula periodic table for benzenoid polycyclic aromatic hydrocarbons (table 1). Second, all possible isomers are enumerated by all combinatorial attachments of $C=CH-CH=C$ units to the immediately preceding row series homologue isomers and by all combinatorial attachments of $C=CH-C=CH-C=C$ or two $C=CH-C$ units to the immediately preceding column homologues (scheme 1). Since the cata-condensed benzenoids have no formula in table 1 above them, the first attachment mode gave the complete set of isomers. Similarly, since many of the strictly peri-condensed benzenoids have no formula in table 1 at their left, either of the second attachment modes gave the complete set of isomers. For benzenoids having formulas located away from the upper or diagonally left sloping boundaries of table 1, all attachment modes were needed to generate all the isomers; duplicates had to be discarded for those benzenoids having inner located formulas. Strictly peri-condensed benzenoid isomers having formulas in table 1 with no formulas either immediately above or to their left were generated



Scheme 1. Recursive aufbau construction of benzenoid hydrocarbons.

attaching a $C=C$ unit to a bay region of the benzenoid structures having a formula located diagonally to the upper right (scheme 1). For example, attachment of a $C=C$ unit to the bay region of benzo[*ghi*]perylene ($C_{22}H_{12}$) gives coronene ($C_{24}H_{12}$). For benzenoid structures having inner table 1 formulas, this latter attachment mode led to no new isomers. Also, no new isomers were generated by attaching the following unit to the bay region of a benzenoid having a formula immediately above the target enumeration formula [7]. In a formal sense, the formulas of C_2H_4 (ethene) and C_6H_6



(benzene) might be considered $N_{Ic} = 0$ row members of table 1, since the aufbau attachment of a C_4H_2 unit to C_2H_4 gives C_6H_6 and another successive attachment of C_4H_2 gives $C_{10}H_8$ (naphthalene).

One benzenoid growth mechanism involves acetylene addition to bay regions. As the simplest example, the main route to benzenoids in benzene pyrolysis is the formation of biphenyl by addition of phenyl to benzene, followed by sequential addition of two acetylene molecules concomitant with the loss of two H_2 to form pyrene, the smallest strictly peri-condensed benzenoid [23]. In general, strictly peri-condensed benzenoids have formulas on the left-hand side staircase-like diagonal of table 1, are without abutting bay regions on their perimeters, and have a minimum number of bay regions for a given number of carbons (N_C); pyrene, coronene, ovalene, and their circum-benzenoid derivatives have no bay regions. Thus, acetylene addition growth of strictly peri-condensed benzenoids is topologically thwarted relative to other peri-condensed benzenoids. It should be noted that this acetylene growth process is equivalent to the aufbau attachment of a C_2 unit to the bay region of a benzenoid hydrocarbon.

The elementary aufbau units are C_2 , C_3H , and C_4H_2 [7]. All other aufbau units are appropriate combinations of these. A rudimentary construction of a new benzenoid from another involves attaching a C_2 unit to a bay region, two C_3H units to two vee regions, or a C_4H_2 unit to an edge of a precursor benzenoid. Consecutive attachment of a C_2 unit to a bay region followed by attaching a C_4H_2 to the edge generated is equivalent to attaching a benzo C_6H_2 unit to a bay region, and attaching three consecutive C_4H_2 units can be made equivalent to attaching a biphenyl $C_{12}H_6$ to an edge of a benzenoid [7].

Some aspects of our aufbau construction process were previously proposed in the excellent thermodynamic work of Stein [24]. Stein used successive C_4H_2 edge and C_2 bay region attachments to trace the most thermodynamically favorable high temperature PAH6 polymerization route for coronene, circumcoronene, etc. [24]. Here, we note that successive C_4H_2 edge and C_2 bay region attachments are, in some examples, equivalent to our $C=CH-C=CH-C=C$ attachment. According to Stein's work, the smallest soot particle corresponds to hexacircum(30, 42, 54, 66, 78, 90)coronene ($C_{384}H_{48}$). For a given number of carbons, strictly peri-condensed benzenoids are among the more stable ones. This is a generalization of Stein's results. This paper by Stein [24] also showed that for direct benzene polymerization, essentially strain-free total resonant sextets were thermodynamically favored. Thus, it is now apparent that our aufbau construction process may be related to the mechanism of pyrolysis, and a premise implied in our work is that our enumeration process, which follows the thermodynamics of the structures being generated, will also be the more efficient one. Indubitably, it is the one of greatest interest and utility to experimental chemists.

Essentially strain-free total resonant sextets were enumerated by attachment of the above C_6H_2 unit to a bay region (scheme 1) or by attachment of a $C_{12}H_6$ biphenyl unit to a sterically unencumbered perimeter edge of a smaller total resonant sextet benzenoid [13,14]; this latter attachment mode is equivalent to attaching three successive C_4H_2 units in a manner which duplicates the biphenyl arrangement. We end this section with a quote from the work of Trinajstić and coworkers [15]:

“The Dias (aufbau/table 1) method obviously becomes very complicated for systems with many isomeric forms because of the enormous combinatorial possibilities. However, if combined with our computer procedure, it can be used for an efficient generation of all isomeric . . . benzenoid hydrocarbons of a particular CH composition”.

5. Excised internal structure concept

Like the aufbau principle, the excised internal structure concept was precluded by spectroscopic methods, by Platt's perimeter rule [25] for cata-condensed benzenoids, and the subsequent spectroscopic distinction of the insular orbitals in peri-condensed benzenoids [26]. Excising the insular structure out from peri-condensed benzenoids and studying the conserved properties and uses of the corresponding excised internal structures in enumeration was made by Dias [9].

The excised internal structure of a benzenoid hydrocarbon consists of all its connected internal third-degree vertices that remain after stripping off all the peripheral carbon vertices. A strictly peri-condensed benzenoid hydrocarbon has no cata-condensed appendages or disconnected internal vertices. Benzo[*a*]pyrene and perylene are not strictly peri-condensed because the former has a cata-condensed appendage (the benzo moiety) and the latter has disconnected internal vertices. Pyrene is a strictly peri-condensed benzenoid with an ethene excised internal structure (table 2). 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 : *s-cis*-1, 3-butadiene, *s-trans*-1, 3-butadiene, and trimethylenemethane diradical (fig. 1). If an 18-carbon-atom perimeter is circumscribed about each of these C_4H_6 isomers with the 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 (table 2). If these three latter strictly peri-condensed benzenoids are circumscribed by a 30-carbon-atom perimeter followed by incrementation with six hydrogens, 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, as well as all benzenoids built up from these cores by attaching successive C_4H_2 units in an aufbau fashion. Thus, the concept of excised internal structure has been useful in a simplified enumeration of benzenoids and in the identification of one type of non-Kekuléan benzenoid species.

If a benzenoid excised internal structure is 1-factorable, 2-factorable, strictly peri-condensed, has one or more bay regions, and/or has one or more selective lineations, then the corresponding larger daughter PAH6 structure formed by circumscribing a perimeter of carbon atoms around the excised internal structure and incrementing it with six hydrogens will also have these attributes [27].

Table 2

Constant isomer series of even strictly peri-condensed benzenoids

Series	Number of isomers	Series	Number of isomers
$C_{10}H_8$	1	$C_{40}H_{16}$	3(1)
$C_{32}H_{14}$		$C_{78}H_{22}$	
$C_{66}H_{20}$		$C_{128}H_{28}$	
$C_{112}H_{26}$...	
$C_{170}H_{32}$		$C_{50}H_{18}$	7(2)
...		$C_{92}H_{24}$	
$C_{16}H_{10}$	1	$C_{146}H_{30}$	
$C_{42}H_{16}$...	
$C_{80}H_{22}$		$C_{62}H_{20}$	12(4)
$C_{130}H_{28}$		$C_{108}H_{26}$	
...		$C_{166}H_{32}$	
$C_{22}H_{12}$	2(1)*	$C_{236}H_{38}$	
$C_{52}H_{18}$...	
$C_{94}H_{24}$		$C_{76}H_{22}$	12(4)
$C_{148}H_{30}$		$C_{126}H_{28}$	
...		$C_{188}H_{34}$	
$C_{24}H_{12}$	1	...	
$C_{54}H_{18}$		$C_{90}H_{24}$	27(12)
$C_{96}H_{24}$		$C_{144}H_{30}$	
$C_{150}H_{30}$		$C_{210}H_{36}$	
...		...	
$C_{30}H_{14}$	3(1)	$C_{106}H_{26}$	38(19)
$C_{64}H_{20}$		$C_{164}H_{32}$	
$C_{110}H_{26}$		$C_{234}H_{38}$	
$C_{168}H_{32}$...	
...			

*The number of less stable diradical isomers are given in parentheses.

6. Summary

In summary, the aufbau principle, the excised internal structure concept, and the concept of strictly peri-condensed benzenoid were evolved in conjunction with the formula periodic table for enumeration of benzenoids (table 1) and represent new ideas formulated by the author. These fundamentals led to the first examples of enumeration of strictly peri-condensed, non-Kekuléan, and total resonant sextet (all-benzenoid systems) benzenoid groups which are of potential interest to experimental chemists [23,24], and the periodic table is one very helpful device for this purpose [28].

This review is ended with the same acknowledgement that appears in *Handbook of Polycyclic Hydrocarbons*, Part B [29].

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Appendix

Glossary of terms

- a_4 – fourth coefficient of the characteristic polynomial;
- a_6 – sixth coefficient of the characteristic polynomial;
- d_s – net tree disconnections of internal graph edges (positive values) or connections (negative values – called negative disconnection);
- n_0 – number of bay regions;
- 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 or carbon vertices;
- 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.

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