Formula Periodic Tables—Their Construction and Related Symmetries

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Received July 26, 1995[⊗]

The algorithmic construction of formula periodic tables for polycyclic conjugated hydrocarbons is detailed. The symmetries associated with this construction are identified. The formula periodic table for benzenoids (Table PAH6) exhibits a one-to-one mapping onto the formula periodic table for fluorenoids/fluoranthenoids minus the constant-isomer fluorenoid/fluoranthenoid formulas and the formula periodic table for benzotropyloids/pleiadienoids which has no constant-isomer series. This work is a contribution to the development of a unified structure theory for polycyclic conjugated hydrocarbons.

INTRODUCTION

We will revisit our prior conjecture[1] that the Formula Periodic Table for Benzenoids (Table PAH6) contains all formulas for all polycyclic conjugated hydrocarbon (PCH) structures with ring size distributions that comply with the equation $3r_3 + 2r_4 + r_5 - r_7 - 2r_8 - 3r_9 = 0$ (r_i = no. of rings of size i). For example, the azulenoids ($r_5 = r_7$, $r_6 = 0$) which consist of paired pentagonal/heptagonal rings will only have formulas found in Table PAH6. Representatives of this PCH class include the known pyrene ($C_{16}H_{10}$) isomers,[2] dicyclopenta[*ef,kl*]heptalene (azupyrene), pentaleno[6,1,2-*def*]heptalene, and dicylohepta[*cd,gh*]pentalene. The azulenobenzenoids ($r_5 = r_7$, $r_6 > 0$) is another PCH class having formulas only found in Table PAH6. Known examples of this class include the three benzoazulenes, dibenzo[*a,e*]azulene, tribenzo[*a,e,h*]azulene, the three azulenophenalenes, and naphtho[1,8-*ab*:4,5-*a′b′*]diazulene.[2] The above equation arises as a condition that the general equation,[1,2] $N_{pc} = N_H - 6 + 3r_3 + 2r_4 + r_5 - r_7 - 2r_8 - 3r_9 - ...$, reduces to $N_{pc} = N_H - 6$ where N_{pc} and N_H are the number of peripheral third-degree carbon vertices and hydrogens, respectively.

While presenting our recent results, we will take the opportunity to review and clarify the results of our original paper.[1] In the (semi)algorithmic generation of formula tables for various classes of polycyclic hydrocarbons, our initial studies were deliberatly restricted to the more chemically reasonable structures. First, odd carbon species were ignored. Second, highly strained systems were omitted. In some cases, this latter was matter of judgment. For example, tetrahedradiene (C_4, in Table PAH_3), cubatetraene (C_8, in Table PAH_4), dodecahedradecaene (C_{20} in Table PAH_5 (Table 1)), and closely related structures were deemed too unstable for inclusion. Also, C_4, C_8, and C_{20} are not really hydrocarbons. As things evolved, it subsequently became apparent that the study of less stable and chemically unreasonable species was necessary for comparing and contrasting these structures versus stable ones in order to more fully understand the variables. This led us to investigate the less stable and experimentally unknown odd radical (odd carbon) benzenoids[3] and then the even radical (even carbon) benzenoids.[4] The discovery of fullerenes led us to re-evaluate the assumption that dodecahedradecaene and related structures should be omitted from Table PAH_5 (Table 1).[5] We currently still exclude tetrahedradiene, cubatetraene, and related unstable even carbon species from the relevant tables.

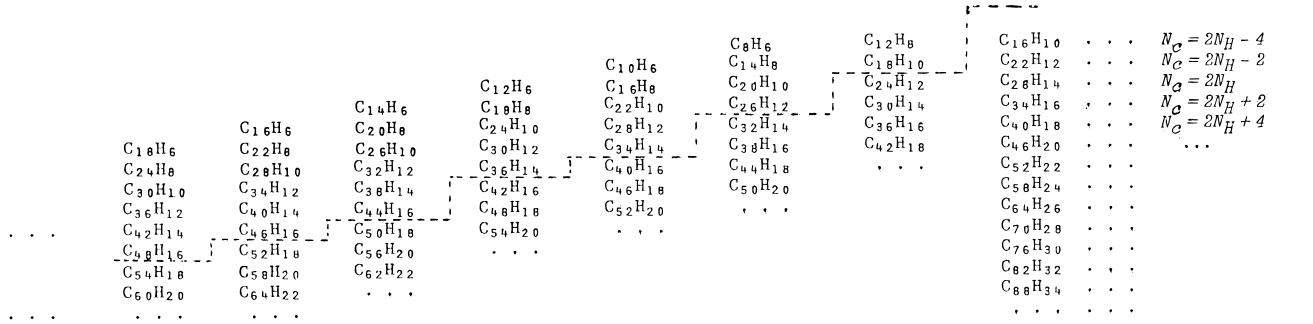
Construction and Organization of the Formula Periodic Tables—Table PAH_5 (Table 1), Table PAH6(odd) (Table 2), and Table PAH_7 (Table 3). For convenience the published tables[1,5]—Table PAH_5 (Table 1), Table PAH6-(odd) (Table 2), and Table PAH_7 (Table 3)—are reproduced herein. The extended version of Table PAH_5 (Table 1) would contain all possible formulas for polypent/polyhex molecular systems.[5] The truncated version given here has been published and only lists the even carbon formulas.[1] To orient the reader note that the sixth column is headed by the formula of pentalene (C_8H_6), and the azupyrene ($C_{16}H_{10}$) isomers referred to in the introduction head the eighth column. Formulas below and to the right of the dashed line in Table PAH_5 (Table 1) can correspond to benzenoid isomeric structures, but formulas above cannot. Formulas corresponding to cata-condensed benzenoids are not found on this table, because no polypent/polyhex molecular system can have these formulas. The maximum number of pentagonal rings that any polypent/polyhex structure with a formula in the first row (the $N_c = 2N_H - 4$ row) of Table PAH_5 (Table 1) can have is two. The maximum number of pentagonal rings is four for formulas in the second row (the $N_c = 2N_H - 2$ row), and so on.

The formula periodic table for benzenoids is referred to as Table PAH6 = Table PAH6(even) U Table PAH6(odd) and is arranged with formulas corresponding to molecular graph structures having the same number of internal third degree vertices (N_{Ic}) in the same row and having the same net disconnections (or connections) (d_s) of internal edges in the same column. This results in the formulas of cata-condensed benzenoids being located in the upper right-hand horizontal edge and the formulas of the constant-isomer benzenoids being located on the left-hand descending staircase edge of Table PAH6. Before our work on odd carbon benzenoids,[3] Table PAH6(even) was referred to as Table PAH6. The formulas on the left-hand staircase of this original table was algorithmically generated by C_2 attachments to bay regions of appropriate precursor structures.[6] For example, C_2 attachment to bay region of naphtho[8,1-*abc*]coronene ($C_{30}H_{14}$) generated ovalene ($C_{32}H_{14}$), the second generation member of the polycircumnaphthalene D_{2h}

[⊗] Abstract published in *Advance ACS Abstracts,* November 1, 1995.

0095-2338/96/1636-0361$12.00/0

Table 1. Formulas of Even Carbon PAHs Having Only Hexagonal and Pentagonal Rings[a]



[a] Benzenoid formulas are located below and to the right of the dashed line.

one-isomer series. Starting with naphthalene, successive attachment of C_4H_2 units in all distinct ways generated all the cata-condensed formulas on the horizontal right-hand edge of Table PAH6. This original work[6] was the first to suggest that in the recursive build-up of benzenoids; only a minimum number of different attachment units should be required. First, we suggested two attachment units, namely C_6H_2 (as two C_3H) and C_4H_2, but later we established that really three were needed for this minimum set; they are C_2, C_3H, and C_4H_2 which were subsequently called elementary aufbau units because all other building-up attachment units must be some composite of these simplest units; this fact alone proves the sufficiency of our aufbau principle for the generation of all benzenoid isomeric structures from these elementary aufbau units.[7] In other words, our corresponding aufbau algorithm is a fundamental building-up principle.[8] Thus, exactly the same method originally used to generate Table PAH6[6] turned out to be applicable in enumerating all benzenoid isomeric structures, without exception. This important idea leads to an enormous reduction of isomorphic (duplicate) structures generated by the enumeration process. The isomorphism problem is common to all algorithms used in the generation of chemical graphs.[9]

Table PAH6(odd) (Table 2) given here has been published.[3] To orient the reader note that phenalenyl ($C_{13}H_9$) in Figure 1 is the smallest odd carbon benzenoid. All benzenoids with formulas in the first row of Table PAH6-(odd) (Table 2) have structures with one internal third degree vertex ($N_{Ic} = 1$), in the second row $N_{Ic} = 3$, and so on. All benzenoid structures with formulas in the same column of Table PAH6(odd) (Table 2) will have the same net disconnection/connection value (d_s) for its internal edges. In Table PAH6 (containing both odd and even carbons), $C_{13}H_9$ ($N_{Ic} = 1$, $d_s = 0$) would be below naphthalene ($C_{10}H_8$, $N_{Ic} = 0$, $d_s = 0$) and above pyrene ($C_{16}H_{10}$, $N_{Ic} = 2$, $d_s = 0$).

The extended version of Table PAH_7 (Table 3) would contain all possible formulas for polyhex/polyhept hydrocarbon molecular systems. The truncated version of Table PAH_7 (Table 3) given here was published previously with three undetected omissions ($C_{38}H_{16}$, $C_{48}H_{18}$, and $C_{60}H_{20}$).[1] While Table PAH_7 (Table 3) given here only lists the even carbon formulas, it is an easy matter to interpolate the odd carbon formulas. To orient the reader pleiadiene ($C_{14}H_{10}$) in Figure 1 is the first formula in the $N_c = 2N_H - 6$ row in Table PAH_7 (Table 3). Formulas below and to the right of the dashed line in Table PAH_7 (Table 3) can correspond to benzenoid isomeric structures, but formulas above cannot.

Symmetries Associated with the Construction of Formula Periodic Tables. The above equations (first paragraph in the Introduction) reveal a symmetry present in the construction of other formula periodic tables. We will first show that the ... $-r_5 + r_7$ ... portion of these equations implies a type of inverse symmetry by comparing the even carbon versions of Table PAH_5 (Table 1) and Table PAH_7 (Table 3) with the odd carbon version of Table PAH6 (Table 2). Recall that Table PAH_5 (Table 1) contains all formulas which correspond to PCH structures having only hexagonal and/or pentagonal rings ($r_6 \geq 0$, $r_5 \geq 1$), and Table PAH_7 (Table 3) contains all formulas which correspond to PCH structures having only hexagonal and/or heptagonal rings ($r_6 \geq 0$, $r_7 \geq 1$). The full Table PAH_5 (Table 1) has a right-hand horizontal edge consisting of formulas ($C_{1+4r}H_{3+2r}$, r = no. of rings) belonging to cata-condensed fluorenoids (fluorenoids have one pentagonal ring and an odd number of carbons) which can be generated from the right-hand horizontal edge of Table PAH6 by subtracting CH from the cata-condensed benzenoid formulas ($C_{2+4r}H_{4+2r}$, r = no. of rings). Subtracting CH corresponds to perimeter-hexagonal-to-pentagonal ring contraction (Figure 1). Generation of the left-hand edge of Table PAH_5 (Table 1) is more complicated.[5] The reverse is true for Table PAH_7 (Table 3). Generation of the right-hand region of Table PAH_7 (Table 3) is more complicated; whereas the left-hand staircase edge of Table PAH_7 (Table 3) can be generated by adding a CH to all left-hand staircase formulas of Table PAH6. Adding CH corresponds to perimeter-hexagonal-to-heptagonal ring expansion (Figure 1). While some benzenoid formulas can correspond to structures composed exclusively of pentagonal rings, no benzenoid formula can correspond to a structure composed of exclusively heptagonal rings. Recall that all benzenoid structures having formulas in or to the left of the $d_s = -2$ column in Table PAH6 can be converted to polypentagonal systems because $N_{Ic}(\text{PAH6}) \geq r$.[5,10] For example, ovalene ($C_{32}H_{14}$, $N_{Ic} = r = 10$) can be converted into the cata-condensed polypent system shown in Figure 2 and is the smallest benzenoid fulfilling this condition. The smallest even carbon polypheptagonal systems are given in Figure 2 all of which have formulas above the horizontal dashed line in Table PAH_7 (Table 3). The leading formula to each row of the upper right-hand boundary of Table PAH_7 (Table 3) is given by $C_{2+5r}H_{4+3r}$ (r = no. of rings) which is the general expression for the formulas of cata-condensed polyheptagonal systems.

Table 2. Formula Periodic Table for Odd Benzenoid PAHs

d_s=−8	d_s=−7	d_s=−6	d_s=−5	d_s=−4	d_s=−3	d_s=−2	d_s=−1	d_s=0	d_s=1	d_s=2	d_s=3	d_s=4	d_s=5	d_s=6	N_{Ic}
. . .								$C_{13}H_9$	$C_{17}H_{11}$	$C_{21}H_{13}$	$C_{25}H_{15}$	$C_{29}H_{17}$	$C_{33}H_{19}$	$C_{37}H_{21}$	. . . 1
								$C_{19}H_{11}$	$C_{23}H_{13}$	$C_{27}H_{15}$	$C_{31}H_{17}$	$C_{35}H_{19}$	. . .		3
								$C_{25}H_{13}$	$C_{29}H_{15}$	$C_{33}H_{17}$	. . .	. . .			5
							$C_{27}H_{13}$	$C_{31}H_{15}$	. . .						7
							$C_{33}H_{15}$	. . .							9
						$C_{35}H_{15}$	. . .								11
						$C_{41}H_{17}$									13
					$C_{37}H_{15}$	. . .									15
					$C_{43}H_{17}$										17
				$C_{45}H_{17}$	. . .										19
			$C_{47}H_{17}$	. . .											21
			$C_{53}H_{19}$	. . .											23
		$C_{55}H_{19}$	. . .												25
	$C_{57}H_{19}$	. . .													27
$C_{59}H_{19}$	. . .														. . .
. . .															. . .

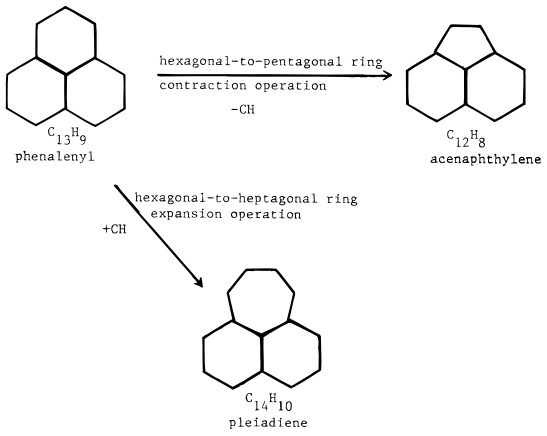


Figure 1. Hexagonal ring contraction and expansion operations for generating and enumerating fluoranthenoids and pleiadienoids.

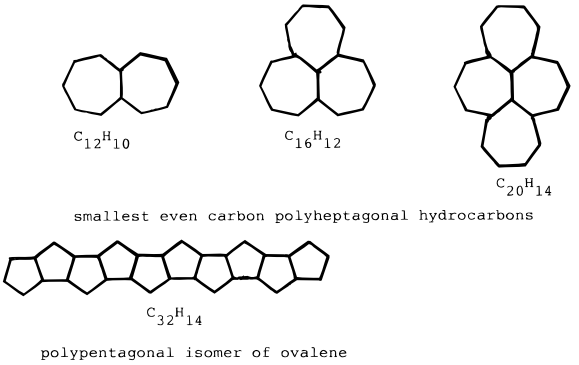


Figure 2. Smallest polypentagonal and polyheptagonal hydrocarbons.

Now consider Table PAH5,6(F/F), the formula periodic table for fluorenoids/fluoranthenoids ($r_6 > 0$, $r_5 = 1$),[11,12] which is a subset of Table PAH_5 (Table 1). Table PAH5,6-(F/F) and Table PAH_5 (Table 1) have the same right-hand horizontal edge, but now the left-hand staircase edge is generated by subtracting CH from all the left-hand staircase edge formulas of Table PAH6 and then including the formulas corresponding to the constant-isomer fluorenoids/fluoranthenoids.

Adding CH to all the formulas in Table PAH6 will generate all formulas for polycyclic conjugated systems possessing one heptagonal ring among otherwise hexagonal ones [Table PAH6,7(B/P) = Table PAH6,7(B) U Table PAH6,7(P)]. This table has the same left-hand edge as Table PAH_7 (Table 3) but otherwise differs for the right-hand edge. The smallest even carbon member of this table is pleiadiene ($C_{14}H_{10}$, cylohepta[*de*]naphthalene), and the smallest odd carbon member is benzotropyl ($C_{11}H_9$). We refer to PCHs having a single heptagonal ring fused to hexagonal ones as benzotropyloids if they possess an odd number of carbons (B means odd) and pleiadienoids if they possess an even number of carbons (P means even). The total formula edge of Table PAH6,7(B/P) is generated by adding CH to all edge formulas of Table PAH6.

In summary, $+r_5 - r_7$ implies a type of inverse symmetry as follows. (a) In enumeration and generation, plus in this equation means contract (−CH) and minus means expand (+CH) a hexagonal ring. (b) The structures on the right-hand horizontal edge of Table PAH_5 (Table 1) and Table PAH5,6(F/F) are identical, have only one pentagonal ring fused to hexagonal ones, and are cata-condensed. The left-

Table 3. Formulas of Even Carbon PAHs Having Only Hexagonal and Heptagonal Rings[a]

																			$C_{42}H_{28}$	$C_{46}H_{30}$	...		$N_c=2N_H-14$
																		$C_{32}H_{22}$	$C_{36}H_{24}$	$C_{40}H_{26}$	$C_{44}H_{28}$	$C_{48}H_{30}$	$C_{52}H_{32}$	$C_{56}H_{34}$	...	$N_c=2N_H-12$
												$C_{22}H_{16}$	$C_{26}H_{18}$	$C_{30}H_{20}$	$C_{34}H_{22}$	$C_{36}H_{24}$	$C_{42}H_{26}$	$C_{46}H_{28}$	$C_{50}H_{30}$	$C_{54}H_{32}$	...	...		$N_c=2N_H-10$
								$C_{12}H_{10}$	$C_{16}H_{12}$	$C_{20}H_{14}$	$C_{24}H_{16}$	$C_{28}H_{18}$	$C_{32}H_{20}$	$C_{36}H_{22}$	$C_{40}H_{24}$	$C_{44}H_{26}$	$C_{48}H_{28}$	$C_{52}H_{30}$	$C_{56}H_{32}$	$C_{60}H_{34}$	...			$N_c=2N_H-8$
								$C_{14}H_{10}$	$C_{18}H_{12}$	$C_{22}H_{14}$	$C_{26}H_{16}$	$C_{30}H_{18}$	$C_{34}H_{20}$	$C_{38}H_{22}$	$C_{42}H_{24}$	$C_{46}H_{26}$	$C_{50}H_{28}$	$C_{54}H_{30}$	$C_{58}H_{32}$	$C_{62}H_{34}$	$C_{66}H_{36}$	...			$N_c=2N_H-6$
								$C_{20}H_{12}$	...	...	...	...	...	...	...	...	...	...	...	...				$N_c=2N_H-4$
								$C_{26}H_{14}$																$N_c=2N_H-2$
								$C_{28}H_{14}$	$C_{32}H_{16}$															$N_c=2N_H$
								$C_{34}H_{16}$	$C_{38}H_{18}$															$N_c=2N_H+2$
							$C_{26}H_{16}$	$C_{40}H_{18}$	$C_{44}H_{20}$															$N_c=2N_H+4$
						$C_{38}H_{16}$	$C_{42}H_{18}$	$C_{46}H_{20}$	$C_{50}H_{22}$															$N_c=2N_H+6$
						$C_{44}H_{18}$	...	$C_{52}H_{22}$	$C_{56}H_{24}$															$N_c=2N_H+8$
				$C_{46}H_{18}$	$C_{50}H_{20}$			$C_{58}H_{24}$	$C_{62}H_{26}$															$N_c=2N_H+10$
			$C_{48}H_{18}$	$C_{52}H_{20}$	...			$C_{64}H_{26}$	$C_{68}H_{28}$															$N_c=2N_H+12$
			$C_{54}H_{20}$	...				$C_{70}H_{28}$	$C_{74}H_{30}$															$N_c=2N_H+14$
		$C_{56}H_{20}$						$C_{76}H_{30}$	$C_{80}H_{32}$															$N_c=2N_H+16$
	$C_{58}H_{20}$	$C_{62}H_{22}$						$C_{82}H_{32}$	$C_{86}H_{34}$															$N_c=2N_H+18$
$C_{60}H_{20}$	$C_{64}H_{22}$							$C_{88}H_{34}$	$C_{92}H_{36}$															$N_c=2N_H+20$
$C_{66}H_{22}$	$C_{70}H_{24}$							$C_{94}H_{36}$	$C_{98}H_{38}$															$N_c=2N_H+22$
$C_{72}H_{24}$	$C_{76}H_{26}$							$C_{100}H_{38}$	$C_{104}H_{40}$															$N_c=2N_H+24$
$C_{78}H_{26}$	...							$C_{106}H_{40}$	$C_{110}H_{42}$															$N_c=2N_H+26$
$C_{84}H_{28}$								$C_{112}H_{42}$	$C_{116}H_{44}$															$N_c=2N_H+28$
$C_{90}H_{30}$								...	...															$N_c=2N_H+30$
...																								$N_c=2N_H+32$
																								$N_c=2N_H+34$
																								$N_c=2N_H+36$
																								$N_c=2N_H+38$
																								$N_c=2N_H+40$
																								$N_c=2N_H+42$
																								$N_c=2N_H+44$
																								$N_c=2N_H+46$
																								$N_c=2N_H+48$

[a] Benzenoid formulas are located below and to the right of the dashed line.

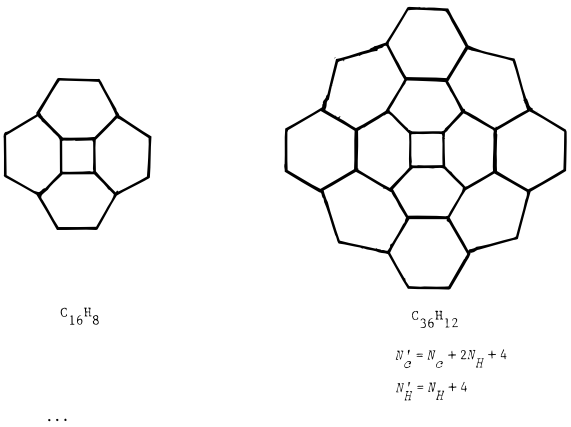


Figure 3. The first two members of the unique biphenylenoid one-isomer series with corresponding formulas not found in Table PAH5,6(I) for indacenoids.

hand staircase edge of Table PAH 5,6(F/F) contains constant-isomer fluorenoids/fluoranthenoids, while the left-hand edge of Table PAH_7 (Table 3) and Table PAH6,7(B/P) are identical, have only one heptagonal ring fused to hexagonal ones, and are strictly peri-condensed. (c) No benzenoid formula can correspond to a polyheptagonal structure, but many benzenoid formulas do correspond to polypentagonal structures (Figure 2). (d) Upon subtraction or addition of CH odd carbon benzenoids beget fluoranthenoids or pleiadienoids and even ones beget fluorenoids or benzotropyloids, respectively. (e) Relative to Table PAH6, Table PAH_5 (Table 1) and Table PAH5,6(F/F) expand in formulas to the left, and Table PAH_7 (Table 3) and Table PAH6,7(B/P) expand in formulas to the right.

In analogy, the horizontal right-hand edges to Table PAH_4 and Table PAH_3 are generated by substracting C_2H_2 and C_3H_3 (from single rings), respectively, from the formulas in the right-hand edge of Table PAH6. Similarly, the left-hand staircase edges to Table PAH_8 and Table PAH_9 are generated by adding C_2H_2 and C_3H_3, respectively, to the formulas in the staircase edge of Table PAH6. Adding C_2H_2 or C_3H_3 to all the edge formulas (both the left-hand and right-hand) of Table PAH6 will generate the formula periodic tables consisting of one octagonal or nonagonal ring, respectively, fused to hexagonal ones; the former is isomorphic to one published by the Cyvin group.[13] The right-hand edge of Table PAH_8 and Table PAH_9 are defined by the formulas corresponding to the cata-condensed polyoctagonal and polynonagonal systems, respectively. The formula periodic table for indacenoids ($r_6 > 0$, $r_5 = 2$),[14] Table PAH5,6(I), can be generated by subtracting C_2H_2 (one CH from two different rings) from all the formulas in Table PAH6 and supplementing with constant-isomer indacenoid formulas.

For PCHs containing a mix of ring sizes, we postulate the following. All formulas of PCH structures obeying one of the three equalities $2r_4 + r_5 - r_7 - 2r_8 = 1$, 0, or -1 will be found on Table PAH5,6(F/F), Table PAH6, or Table PAH6,7(B/P), respectively, but not necessarily all inclusively. This latter proviso is illustrated by the following example for $2r_4 + r_5 - r_7 - 2r_8 = 2$. Table PAH5,6(I)[14] is a subset of the formula periodic table for biphenylenoids;[15] only the smallest unique one-isomer series (Figure 3) of the latter has formulas absent in the former table. We expect the formulas for other unique one-isomer series belonging to other periodic table classes to also be exceptional. This is an amendment of our original postulate.[1]

Symmetry in the Enumeration and Generation of Fluorenoids/Fluoranthenoids and Benzotropyloids/Pleiadienoids. In our prior work,[11] we evolved for the first time the unique strategy for enumeration and generation of fluorenoids/fluoranthenoids from known benzenoid isomer sets which was subsequently extended toward enumeration of indacenoids.[14] This strategy was simply to take all combinatorial perimeter-hexagonal-to pentagonal ring contractions to all the members of a benzenoid isomer set. This strategy was sufficient for benzenoids having less than five internal third degree vertices. For five or more internal third degree vertices, one needed to supplement the enumerations by deployment of the excised internal structure concept.[16]

The first examples of enumeration benzotropyloids and pleiadienoids (C_7H_7-1, $C_{11}H_9$-1, $C_{14}H_{10}$-1, $C_{15}H_{11}$-4, $C_{17}H_{11}$-2, $C_{19}H_{13}$-13) were accomplished by Zahradnik and Pancir.[17] More recently Cyvin and co-workers[18] have deployed my strategy by converting C_nH_s benzenoids to $C_{n+1}H_{s+1}$ monoheptabenzenoids by expanding one of the hexagons at the perimeter to a heptagon. For systems having seven or more internal third degree vertices, the benzotropyloid and pleiadienoid isomers generated in this manner usually had to be supplemented by exploiting my excised internal structure concept. When the ultimate excised internal structure was a strictly peri-condensed benzenoid, no supplemental enumeration was necessary, even though the number of internal third degree vertices exceeded seven.[18]

Criteria for Classifying as a Periodic Table Set. The question that we like to address in this section is whether all the tables discussed herein are just formula tables or formula periodic tables. A periodic table set has been defined as a large to infinite, two-dimensional, partially ordered set obeying Dobereiner's triad principle, with any central element having a metric property that is the arithmetic mean of two flanking elements. It is a well ordered set in that it must possess a least element a smallest member.[19] A periodic table set displays hierarchical ordering of the elements and edge effects. By edge effect, we mean that elements on the boundary edge of the table will exhibit more exceptional characteristics or behavior. First, we like to point out that all the tables discussed here have been derived from Table PAH6 which has been established as being a periodic table set.[19] This in itself suggests that they must be periodic table sets. But let us address this further by examining the edge effect characteristic.

All the tables discussed have cata-condensed structures on located their right-hand boundary edge. Cata-condensed structures as a general rule are characteristically unique. The left-hand staircase boundary edge possess strictly peri-condensed structures. Tables PAH_3, Table PAH_4, Table PAH_5 (Table 1), Table PAH5,6(F/F), and Table PA5H,6(I) have cata-condensed structures on the right-hand edge that contain only one trigonal, tetragonal, and pentagonal ring, respectively. Also, the latter two tables have constant-isomer series on their left-hand edges.[11,14] The left-hand edge of Table PAH_5 (Table 1) has been shown to be bounded by the fullerenes.[5] The structures on the left-hand edge of Table PAH_7 (Table 3), Table PAH_8, and Table PAH_9 only possess one heptagonal, octagonal, and nonagonal ring, respectively. The right-hand (staircase) edges of Table PAH_7 (Table 3), Table PAH_8, and Table PAH_9 are defined by the leading row formulas associated with cata-condensed polyheptagonal, polyoctagonal, and polynonagonal structures, respectively.

All these tables exhibit hierarchical ordering where they sort the formulas into structure regimes. In all cases, as one moves from left to right in a row or from top to bottom in a column the corresponding structures increase in size and number of isomers. Our conclusion is that all the tables discussed herein are formula periodic tables.

CONCLUSION

The algorithmic generation of Table PAH6 used three increments (C_2, C_3H, and C_4H_2) which turned out to be the essence of our fundamental aufbau principle that reduces, but not eliminates, the isomorphism problem in the generation of benzenoid chemical graphs. Using Table PAH6 and the corresponding benzenoid (polyhex) structures, subtracting CH, which equates to perimeter-hexagonal-to-pentagonal ring contraction, leads to the right-hand horizontal edge of Table PAH5,6(F/F) and the corresponding fluorenoids/fluoranthenoids.[11] Similarly, adding CH, which equates to perimeter-hexagonal-to-heptagonal ring expansion, leads to Table PAH6,7(B/P) and the corresponding benzotropyloids/pleiadienoids.[18] These and numerous other results are made possible because an inherent symmetry in the formula/structure content of Table PAH6 exists. There is a one-to-one mapping of Table PAH6 with Table PAH5,6(F/F) minus the fluorenoid/fluoranthenoid constant-isomer formulas and Table PAH6,7(B/P) (which has no constant-isomer series[13]) but not with Table PAH_5 (Table 1) and Table PAH_7 (Table 3).

REFERENCES AND NOTES

(1) Dias, J. R. Periodic Table for Polycyclic Aromatic Hydrocarbons. 2. Polycyclic Aromatic Hydrocarbons Containing Tetragonal, Pentagonal, Heptagonal, and Octagonal Rings. *J. Chem. Inf. Comput. Sci.* **1982**, *22*, 139−152.

(2) Dias, J. R. Polycyclic Hydrocarbons, Part B; Elsevier: New York, 1988.

(3) Dias, J. R. A Periodic Table for Polycyclic Aromatic Hydrocarbons. Part IX. Isomer Enumeration and Properties of Radical Strictly Peri-Condensed Polycyclic Aromatic Hydrocarbons. *J. Mol. Struct. (Theochem)* **1986**, *137*, 9−29.

(4) Dias, J. R. Constant-Isomer Benzenoid Series and Their Polyradical Subsets. *Theor. Chim. Acta* **1991**, *81*, 125−138.

(5) Dias, J. R. Deciphering the Information Content of Polycyclic Conjugated Hydrocarbon Formulas − From Benzenoids to Fullerenes. *Tetrahedron* **1993**, *49*, 9207−9220.

(6) Dias, J. R. A Periodic Table for Aromatic Hydrocarbons. Isomer Enumeration of Fused Polycyclic Aromatic Hydrocarbons. 1. *J. Chem. Inf. Comput. Sci.* **1982**, *22*, 15−22.

(7) Dias, J. R. A Formula Periodic Table for Benzenoid Hydrocarbons and the Aufbau and Excised Internal Structure Concepts in Benzenoid Enumerations. *Z. Naturforsch.* **1989**, *44a*, 765−771. Dias, J. R. A Periodic Table for Benzenoid Hydrocarbons. *Top. Curr. Chem.* **1990**, *153*, 123−143.

(8) Cyvin, S. J.; John, P. E.; Gutman, I.; Brunvoll, J.; Cyvin, B. N. Contributions to the Theory of Benzenoid Isomers. Part 2: Building-up Principles. *J. Mol. Struct. (Theochem)* **1995**, *334*, 243−247.

(9) Bangov, I. P. Toward the Solution of the Isomorphism Problem in Generation of Chemical Graphs: Generation of Benzenoid Hydrocarbons. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 167−173.

(10) Dias, J. R. A Periodic Table for Polycyclic Aromatic Hydrocarbons. *Acc. Chem. Res.* **1985**, *18*, 241−248. Dias, J. R. Notes on Constant-Isomer Series. *J. Chem. Inf. Comput. Sci.* **1993**, *33*, 117−127.

(11) Dias, J. R. Series of Fluorenoid/Fluoranthenoid Hydrocarbons Having a Constant Number of Isomers. *Chem. Phys. Lett.* **1991**, *185*, 10−15, 187, 334. Dias, J. R. Studies in Deciphering the Information Content of Chemical Formulas: A Comprehensive Study of Fluorenes and Fluoranthenes. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 2−11.

(12) Cyvin, S. J. Graph-Theoretical Studies on Fluoranthenoids and Fluorenoids. Part 1. *J. Mol. Struct. (Theochem)* **1992**, *262*, 219−231. Cyvin, S. J.; Cyvin, B. N.; Brunvoll, J. Graph-Theoretical Studies on Fluoranthenoids and Fluorenoids. Part 2. *J. Mol. Struct. (Theochem)* **1993**, *281*, 229−236. Cyvin, S. J.; Cyvin, B. N.; Brunvoll, J.; Fuji, Z.; Xiaofeng, G.; Tosic, R. Graph-Theoretical Studies on Fluoranthenoids and Fluorenoids: Enumeration of Some Catacondensed Systems. *J. Mol. Sruct. (Theochem)* **1993**, *285*, 179−185.

(13) Brunvoll, J.; Cyvin, B. N.; Cyvin, S. J. Mono-Q-Polyhexes with Q Larger than 6: Polygonal Systems Representing a Class of Polycyclic Conjugated Hydrocarbons. *J. Chem. Inf. Comput. Sci.* **1994**, *34*, 903−911.

(14) Dias, J. R. Deciphering the Information Content of Chemical Formulas: Chemical and Structural Characteristics and Enumeration of Indacenes. *J. Chem. Inf. Comput. Sci.* **1992**, *32*, 203−209.

(15) Cyvin, S. J.; Cyvin, B. N.; Bronvoll, J. General Formulations for Some Polycyclic Hydrocarbons. Constant-Isomer Series and a Formula Index. *Chem Phys. Lett.* **1993**, *201*, 273−277.

(16) Dias, J. R. A Formula Periodic Table for Benzenoid Hydrocarbons and the Aufbau and Excised Internal Structure Concepts in Benzenoid Enumerations. *Z. Naturforsch.* **1989**, *44a*, 765−771. Brunvoll, J.; Cyvin, B. N.; Cyvin, S. J.; Gutman, I. *Z. Naturforsch.* **1988**, *43a*, 889−895.

(17) Zahradnik, R.; Pancir, J. HMO Energy Characteristics; IFI/Plenum: New York, 1970.

(18) Cyvin, B. N.; Brendsdal, E.; Brunvoll, J.; Cyvin, S. J. Molecular Vibrations of Heptacirculene and Molecular Topology of Monoheptapolyhexes. *J. Mol. Struct.* **1994**, *327*, 121−130.

(19) Dias, J. R. The Formula Periodic Table Set for Benzenoid Hydrocarbons and the Unifying Theory of a Periodic Table Set. Polycyclic Aromatic Compounds, **1994**, *4*, 87−106. Dias, J. R. Setting Benzenoids to Order. *Chem. Brit.* **1994**, 384−386.

CI9500804