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Correlations and topology of triangular benzenoid hydrocarbons: a comparative study of two series representing the least and most stable benzenoid hydrocarbons[†]

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ABSTRACT: While reviewing aspects of our topological paradigm and the benchmark role played by the benzenoid polyradicals shaped like equilateral triangles, the topological properties of the reactive polyradicals and their stable associated leapfrog total-resonant-sextet benzenoids are studied. Copyright © 2001 John Wiley & Sons, Ltd.

KEYWORDS: triangular benzenoid hydrocarbons; topology; polycyclic aromatic hydrocarbons; leapfrog algorithm

INTRODUCTION

There are two classes of benzenoid hydrocarbons having structures shaped like equilateral triangles (D_{3h}). One class consists of the benzenoid polyradical series (C_nH_s, $n = t^2 + 6t + 6,\ s = 3t + 6,\ t = 1, 2, 3, \ldots$) which starts with the phenalenyl monoradical (Fig. 1), and the other class consists of the benzenoid total-resonant-sextet series ($n = 3t^2 + 9t + 6,\ s = 6t + 6$) which starts with triphenylene (Fig. 2); benzene ($t = 0$) is regarded as the zero-generation member for both series. The members of the radical series are among the least stable benzenoid systems, whereas the members of the total-resonant-sextet series are among the most stable benzenoids. The first two members ($t = 1$ and 2) of both series in Figs 1 and 2 are known chemical species.[1–4] The initial members of these two series were studied as building blocks in nanotube Y-junctions with metallic properties.[5] With regard to Ref. 5, it is interesting to note the jargon used by material scientists compared with what chemists use. For example, the triangular polyradicals in Fig. 1 were said to be metallic, and the number of metallic states (zero eigenvalue degeneracy) is the difference in the starred and unstarred atoms. Triangular benzenoid polyradicals have singly occupied MOs in their energy gaps, and such pπ-conjugated systems are molecular analogues of semiconductors with defect states that could be used in molecular electronics.[5]

Total-resonant-sextet (TRS) benzenoid hydrocarbons have C_nH_s formulas where the number of carbons ($n = N_c$) is divisible by six and $n/6$ sextet rings [r(sextet)]; sextet rings are hexagonal rings within a benzenoid system containing three pπ-bonds that can mutually permute independently of the other conjugated pπ-bonds. The triangular polyradical class have formulas with the number of hydrogens ($s = N_H$) divisible by three, and the triangular TRS class have formulas with the number of hydrogens divisible by six (and three). Using Fowler's leapfrog algorithm,[6] it can be shown that a one-to-one topological correspondence exists between these two classes of D_{3h} benzenoid hydrocarbons. This study was undertaken to understand more fully this correspondence and how it relates simultaneously to both the least stable and the most stable benzenoid structures. Also, our topological understanding of ideal model alternant polycyclic aromatic hydrocarbons (PAHs) is an essential prerequisite for gaining an understanding of nonalternant PAHs and carbon fullerenes.[6]

SOME FUNDAMENTAL STRUCTURAL INVARIANTS

A benzenoid molecular graph is a σ-bond skeleton representation with r fused hexagons, N_c (carbon) vertices, q edges, N_{Ic} internal third-degree vertices (carbon vertices bounded by three hexagonal rings), N_{pc} peripheral third-degree vertices and N_H second-degree vertices. Let t be the generation index. For example, $t = 0$ for benzene and $t = 1$ for phenalenyl (Fig. 1) and triphenylene (Fig. 2). For the triangular polyradical series (Fig. 1), we have

$$N_c = N_{Ic} + N_{pc} + N_H = t^2 + 6t + 6$$

$$N_H = 3t + 6$$

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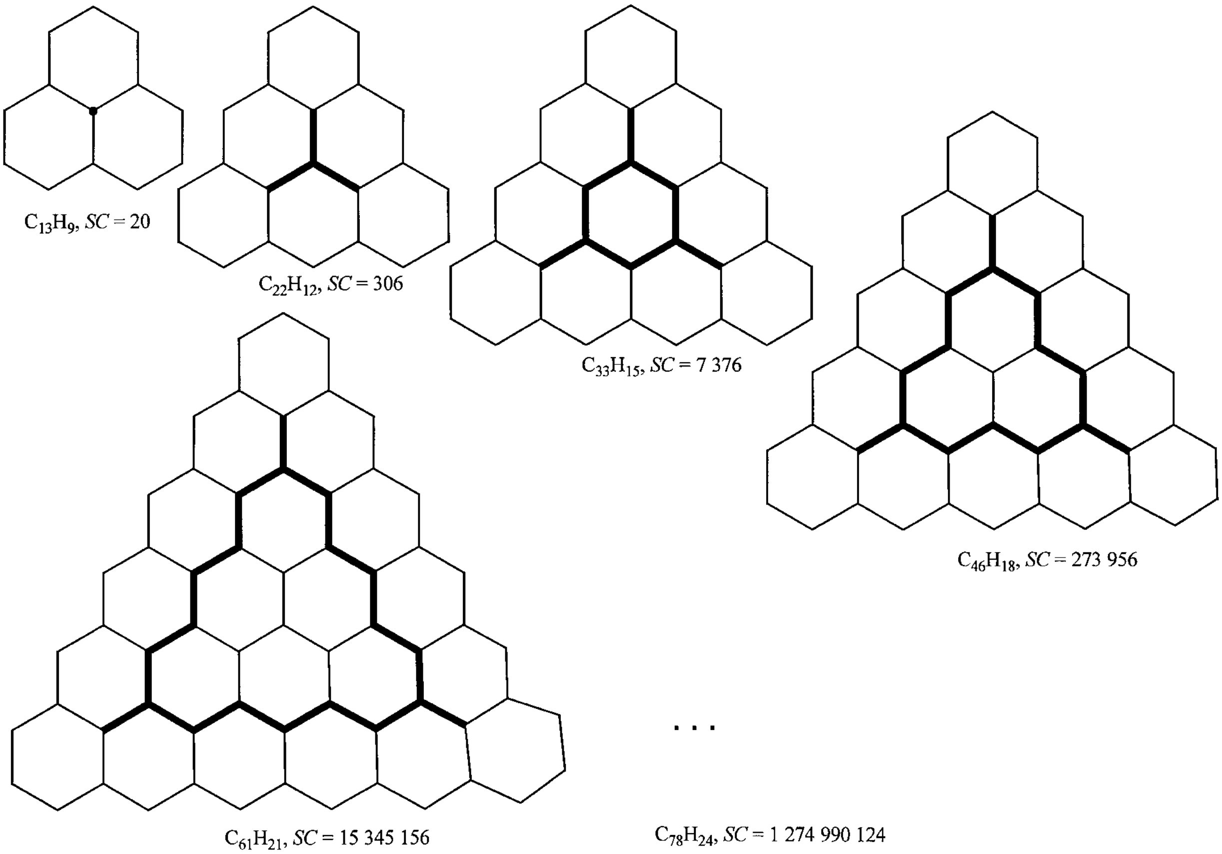


Figure 1. Smallest most condensed members of the benzenoid polyradical series. Their excised internal structures are shown in bold

$$r = \frac{1}{2}(N_c + 2 - N_H) = \frac{1}{2}(t^2 + 3t + 2)$$

$$q = \frac{1}{2}(3N_c - N_H) = \frac{1}{2}(3t^2 + 15t + 12)$$

$$N_{Ic} = t^2$$

$$N_{pc} = N_H - 6 = 3t$$

and for the triangular TRS series (Fig. 2), we have

$$N_c = 3t^2 + 9t + 6$$

$$N_H = 6t + 6$$

$$r = \frac{1}{2}(3t^2 + 3t + 2)$$

$$q = \frac{1}{2}(9t^2 + 21t + 12)$$

$$N_{Ic} = 3t^2 - 3t$$

$$N_{pc} = 6t$$

Graph-theoretically, a total-resonant-sextet (TRS) is a benzenoid with a molecular graph that has a 2-factor (spanning) subgraph composed exclusively of disconnected) hexagon components.[7] The hexagonal rings of a TRS molecular graph can be filled-in with circles in such a way that no two adjacent hexagons will have inscribed circles; these circle-inscribed-hexagons correspond to resonant sextets and all adjacent hexagon are 'empty.'

The inner dual of a benzenoid molecular graph is constructed by putting points in every hexagon and connecting each with lines to every adjacent point. Thus, the inner dual of the molecular graph members to the radical series (Fig. 1) form a series of triangular lattices of increasing size. These triangular lattices correspond to geometric representations of triangular numbers, known to mathematicians, which equals the number of hexagonal rings $r = \frac{1}{2}t(t+1)$ where $t = 1, 2, 3, \ldots$, is the membership generation of the series. The inner dual of the inner dual gives the excised internal structure[8] which is a connected subgraph that contains all the internal third-degree vertices belonging to the original strictly pericondensed benzenoid molecular graph; strictly pericondensed benzenoids have no benzo or catacondensed appendages and have connected excised internal structures. All the triangular benzenoid polyradicals in Fig. 1 are strictly pericondensed but the

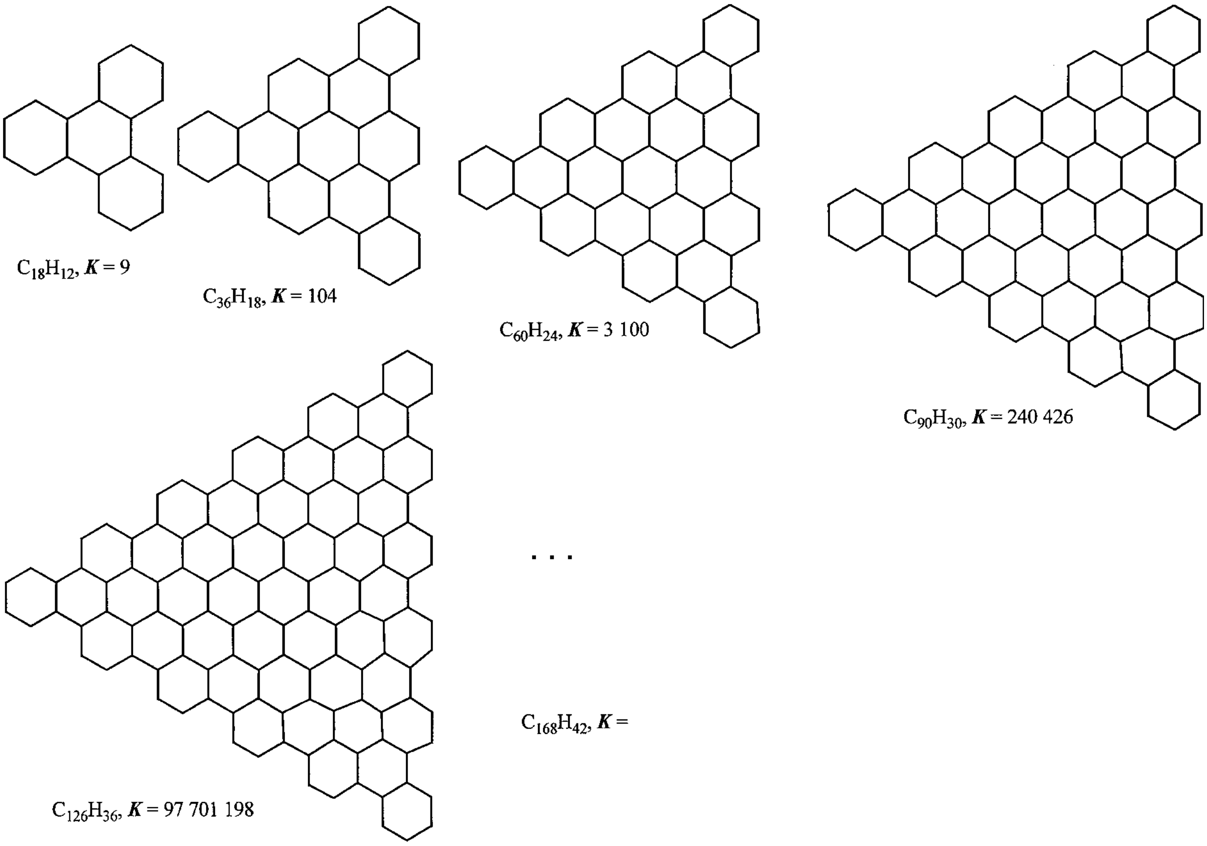


Figure 2. Triangular total resonant sextet benzenoid hydrocarbons and their number of resonance structures (*K*)

TRS benzenoids in Fig. 2 are not because they possess (three) benzo (quarto perimeter regions) appendages. The Wiener index *W* is equal to the sum of the distances between all pairs of vertices of the respective molecular graph.[9] The number of resonance structures of a polyradical (non-Kekulean) benzenoid is designated by *SC*.

LEAPFROG ALGORITHM

The leapfrog of any benzenoid hydrocarbon is a total-resonant-sextet benzenoid. The leapfrog operation consists of the following steps.[6,7] Each hexagonal ring of a benzenoid molecular graph is divided into six equilateral triangles by drawing a line from each of its six vertices to a central point (called omnicapping operation). The central points within each equilateral triangle are joined by lines to neighboring triangles (called inner dual operation). The inscribed graph thus generated corresponds to a molecular graph of a total-resonant-sextet benzenoid. The parent benzenoid (*P*) and successor leapfrog benzenoid (*L*) are called associates. In going from parent to leapfrog the following topological correspondences hold:

$$P(C_nH_s) \rightarrow L(C_{3n-3s+6}H_{2s-6})$$

$$r \rightarrow r(\text{sextet})$$

$$N_{\text{Ic}} \rightarrow r(\text{empty})$$

$$N_{\text{pc}} \rightarrow n_{\text{o}}{}'$$

$$n_i \rightarrow n_{i+1}{}'$$

where the number of internal third degree vertices N_{Ic} becomes the number of empty rings (rings without sextets) *r*(empty), the number of peripheral third-degree vertices N_{pc} becomes the number of bay regions n_0 (perimeter edges with two third-degree vertices) and n_i is the number of perimeter sections with *i* secondary vertices between two peripheral third-degree vertices. Molecular symmetry is preserved by this operation, and all open-shell (radical) parent benzenoid systems become closed-shell (nonradical) leapfrog benzenoid systems. The leapfrog of benzene is benzene (null operation). In the leapfrog conversion of phenalenyl ($C_{13}H_9$) to triphenylene ($C_{18}H_{12}$) in Fig. 3, $N_{\text{Ic}} = r(\text{empty}) = 1$, N_{pc}

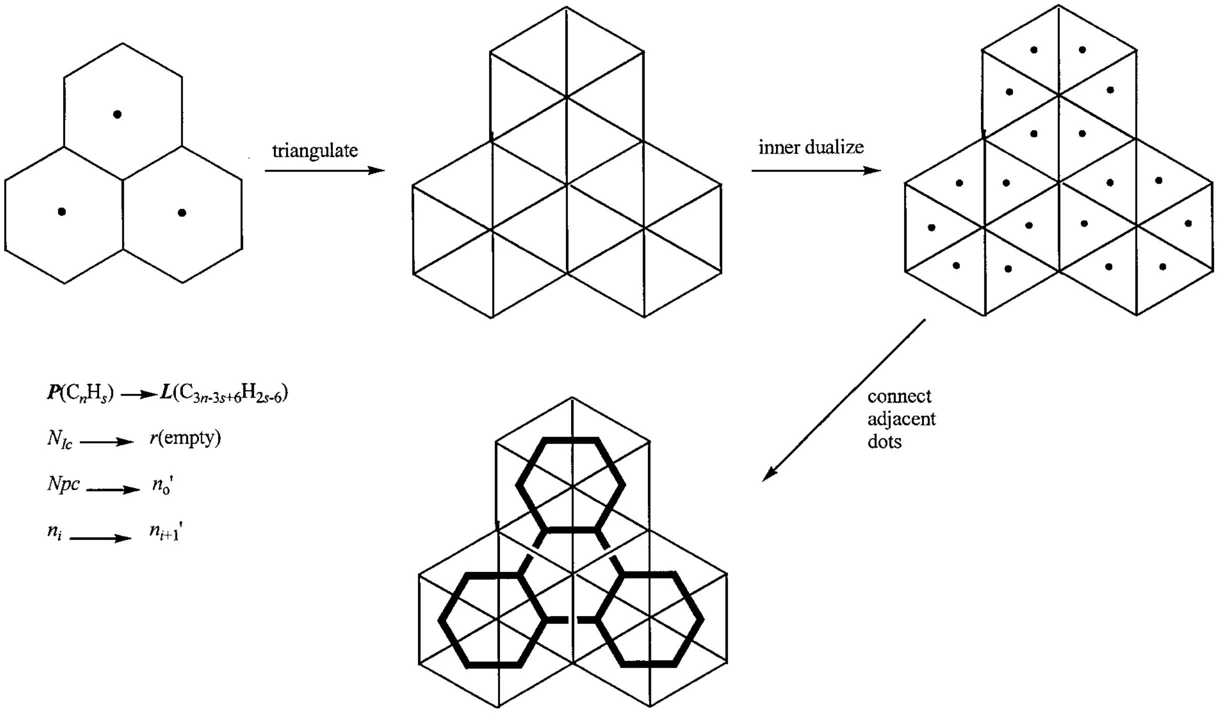


Figure 3. Application of the leapfrog algorithm on phenalenyl monoradical ($C_{13}H_9$) gives triphenylene ($C_{18}H_{12}$)

$= n_0' = 3$, $n_3 = n_4' = 3$ and D_{3h} symmetry is preserved. In general, the rings and internal third-degree vertices in the parent become resonant-sextet rings and empty (additional) rings in the corresponding leapfrog, respectively. Thus, $r(\text{TRS}) = r(\text{sextet}) + r(\text{empty}) = r + N_{\text{Ic}}$, where r and N_{Ic} refer to the precursor (parent) benzenoid system. Whenever members of the series in Fig. 1 are vertex-centrix the leapfrog members in Fig. 2 are ring-centrix.

PROPERTIES OF THE TRIANGULAR BENZENOID POLYRADICAL AND TOTAL-RESONANT-SEXTET SERIES

The members to both series have D_{3h} symmetry, benzene as their zero generation member, at least two-thirds of their eigenvalues doubly degenerate and a large number of resonance structures. All the members of the triangular polyradical series (Fig. 1) have three selective lineations and are consequently triply degenerate in the HMO eigenvalues of ± 1. Starting with the $C_{36}H_{18}$ TRS member (Fig. 2), every other member of the TRS series has three selective lineations and are triply degenerate in the eigenvalues of ± 1.

No TRS formula corresponds to a set of benzenoid isomers which includes a triangular polyradical. Conversely, no (even carbon) triangular polyradical can have a TRS formula. As a consequence of the fact that the inner dual of the inner dual of a strictly pericondensed benzenoid gives its excised internal structure, the excised internal structure of the triangular benzenoid radicals corresponds to the inner dual of the precursor TRS of its associate TRS. For example, the molecular graph of trimethylenemethane diradical is the excised-internal structure of the molecular graph of triangulene ($C_{22}H_{12}$, Fig. 1) and the inner dual of triphenylene ($C_{18}H_{12}$, Fig. 2).

The members of the triangular polyradical series may be odd-or even-carbon species, have no bay perimeter regions, numerous solo regions and three trio regions, are open-shell species and have no one-factor or two-factor subgraphs; whereas the members of the triangular TRS series are always even-carbon species, have numerous bay perimeter regions and three quarto regions, are closed-shell species and have numerous one-factor and two-factor subgraphs. It is well known, other things being equal, that benzenoid solo perimeter regions are the most reactive chemical reaction sites and open-shell species are more reactive than closed-shell species. Similarly, benzenoids with more bay perimeter regions, more sextets, more one-factor (Kekulé structures) and two-factor subgraphs are more stable. These topologically based properties are accumulated in these opposing series and provide a mark contrast.

The empty ring configuration of a triangular TRS has the same shape as the immediately prior TRS in the series of Fig. 2. The most 'empty' of the empty rings is one which is empty for a TRS and its empty ring configuration shaped like the immediately prior TRS. For example, the empty ring configuration of tribenzo[*a*,*g*,*m*]coronene

($C_{36}H_{18}$, Fig. 2) corresponds to triphenylene ($C_{18}H_{12}$) and the central ring in both are empty. The inner dual of the empty ring configuration of the leapfrog coincides with the excised internal structure of the parent where rings replace vertices.

EQUILATERAL TRIANGULAR SHAPE AND ITS RELATIONSHIP TO THE EXCISED INTERNAL STRUCTURE

The radical degree of any benzenoid hydrocarbon is easily determined by its peak-to-valley difference, $|\wedge - \vee|$ = number of unpaired electrons, which for well-behaved benzenoid hydrocarbons coincides with the number of HMO zero eigenvalues.[10] The equilateral triangular shape of the benzenoids in Fig. 1 consisting of solo and trio perimeter regions maximizes the peak-to-valley differences (and radical degree) for the given number of rings. TRS triangular benzenoids have no such shape dependence. The graph formed by the internal vertices of a the molecular graph of a strictly pericondensed benzenoid coincides with its excised internal structure. The excised internal structures for the benzenoid triangular polyradicals are shown in bold in Fig. 1. Polyradical benzenoids with an odd number of unpaired electrons must be odd-carbon species, and polyradicals with an even number of unpaired electrons must even-carbon species. If we exclude concealed benzenoid radical systems, then the following statements must be true.[10] No strictly pericondensed benzenoid with less than four internal-third-degree (N_{Ic} <4) can have a diradical form. Strictly pericondensed benzenoid diradicals must have an excised internal structure which is trimethylenemethane diradical or can be pruned to trimethylenemethane diradical. No strictly pericondensed benzenoid with N_{Ic} <9 can have a triradical form. No strictly pericondensed benzenoid with N_{Ic} <16 can have a tetraradical form. In general, the radical degree per a given minimum number of internal-third-degree vertices for strictly pericondensed benzenoids is given by the triangular polyradicals in Fig. 1.

WIENER NUMBERS OF TRIANGULAR BENZENOID HYDROCARBONS

The Wiener numbers (W) for the benzenoids of the paper were obtained by determining the complete set of elementary cuts per the method Gutman and Klavzar.[9] From these data, exact analytical expressions were determined. For the tth-generation member of the triangular free-radical benzenoids,

$$W(t) = \frac{1}{10}(4t^5 + 60t^4 + 315t^3 + 720t^2 + 731t + 270)$$

and triangular TRS,

$$W(t) = \frac{1}{20}(126t^5 + 945t^4 + 2700t^3 + 3645t^2 + 2304t + 540)$$

Both of these analytical expressions give $W(0) = 27$ for benzene, which is the zero-generation member for both triangular series. It should also be noted that these analytical expressions are to the fifth power consistent with the Wiener number analytical expression for our circumcoronene D_{6h} one-isomer series[11,12] obtained by Gutman and Klavzar.[9]

Various linear regression plots of Wiener number versus ln (SC) for the triangular systems in Fig 1 and 2 were investigated. Here it is assumed that ln (SC) is a measure of resonance energy.[13] Figures 4 and 5 give two examples having correlation coefficients >0.998.

CONSTANT-ISOMER SERIES

Both phenalenyl ($C_{13}H_9$) and triangulene ($C_{22}H_{12}$) are the initial (first-generation, $t = 1$) members of the D_{3h} constant-one-isomer monoradical and diradical series, respectively, generated by successive circumscribing.[14] If one does not distinguish between open-shell or closed-shell characteristics, then triangulene also belongs to the constant-three-isomer benzenoid series shown in Fig. 6. Leapfrogging the first-generation members of the constant-three-isomer benzenoid series gives the first-generation members of the TRS constant-three-isomer series (Fig. 6).

In Fig. 7, triangulene is used as an illustrative example for showing more fully the relationships between the circumscribing of benzenoids, augmented circumscribing of TRS, constant-isomer series and leapfrogging. Circumscribing triangulene once with a carbon chain necklace gives circumtriangulene ($C_{52}H_{18}$), which is the second-generation member ($t = 2$). In general, this process has the formula recursion of $C_nH_s \rightarrow C_{n+2s+6}H_{s+6}$. Augmented circumscribing of a TRS

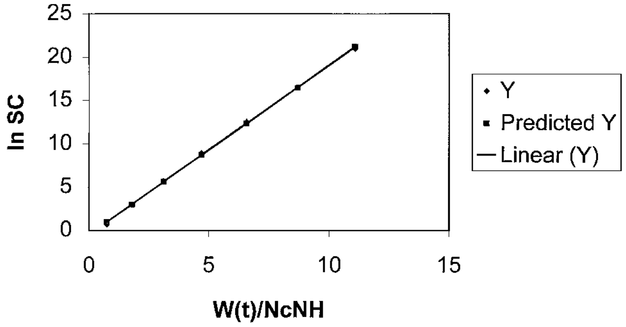


Figure 4. Wiener number versus ln (SC) for triangular poly radicals

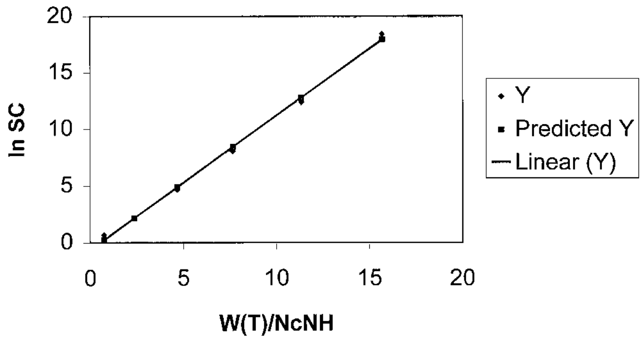


Figure 5. Wiener number versus ln (*SC*) for triangular TRS

benzenoid is illustrated in Fig. 7 by the transformation of tribenzo[*a,g,m*]coronene ($C_{30}H_{18}$), which itself can be formed by leapfrogging triangulene. In augmented circumscribing, all perimeter CHs are first transformed to methylenyl groups and then circumscribed. The formula recursion for augmented circumscribing is $C_nH_s \rightarrow C_{n+3s+18}H_{s+12}$. Thus, the $C_{108}H_{30}$ TRS benzenoid in Fig. 7 can be formed by augmented circumscribing of tribenzo[*a,g,m*]coronene ($C_{36}H_{18}$) or by leapfrogging circumtriangulene ($C_{52}H_{18}$). Performing these transformations repeatedly on the other $C_{22}H_{12}$ benzenoids or TRS $C_{36}H_{18}$ benzenoids in Fig. 6 leads to the respective constant-three-isomer series.

In the case of the three $C_{22}H_{12}$ benzenoids, if one is only interested in the diradical subset, then triangulene turns out to be the first-generation member of the unique diradical D_{3h} constant-one-isomer series.[14] The isomer numbers and corresponding topology of the member benzenoids for all the diradical constant-isomer series match precisely those of the monoradical constant-isomer series of which phenalenyl is the first-generation member of the unique D_{3h} constant-one-isomer series. Furthermore, the triradical, tetraradical, pentaradical, etc., benzenoid subsets follow exactly the same paradigm. Thus, the members of the triangular polyradical series in Fig. 1 serve as benchmarks to the respective constant-isomer polyradical subsets.

Whereas phenalenyl monoradical and triangulene diradical are first-generation members of the respective

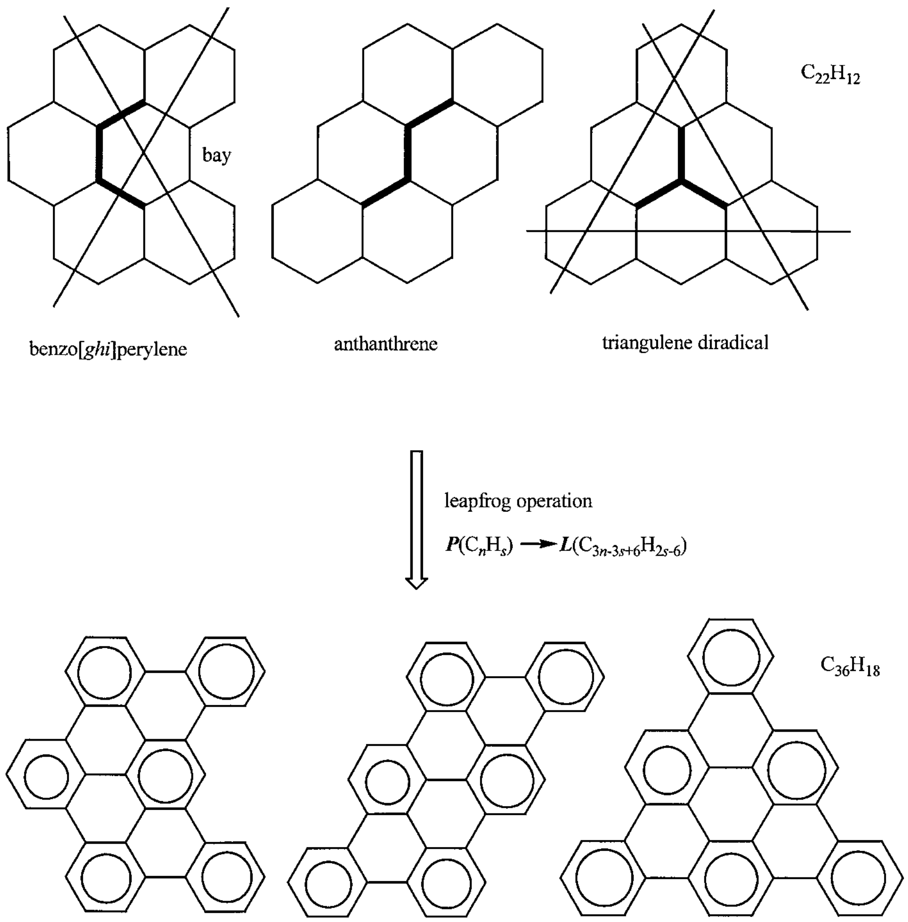


Figure 6. The leapfrog operation on the only three $C_{22}H_{12}$ benzenoids generates the three most stable (total resonant sextet) $C_{36}H_{18}$ benzenoids without knowing what the remaining 413 isomers look like; there are 337 nonradical and 79 diradical $C_{36}H_{18}$ benzenoid isomers

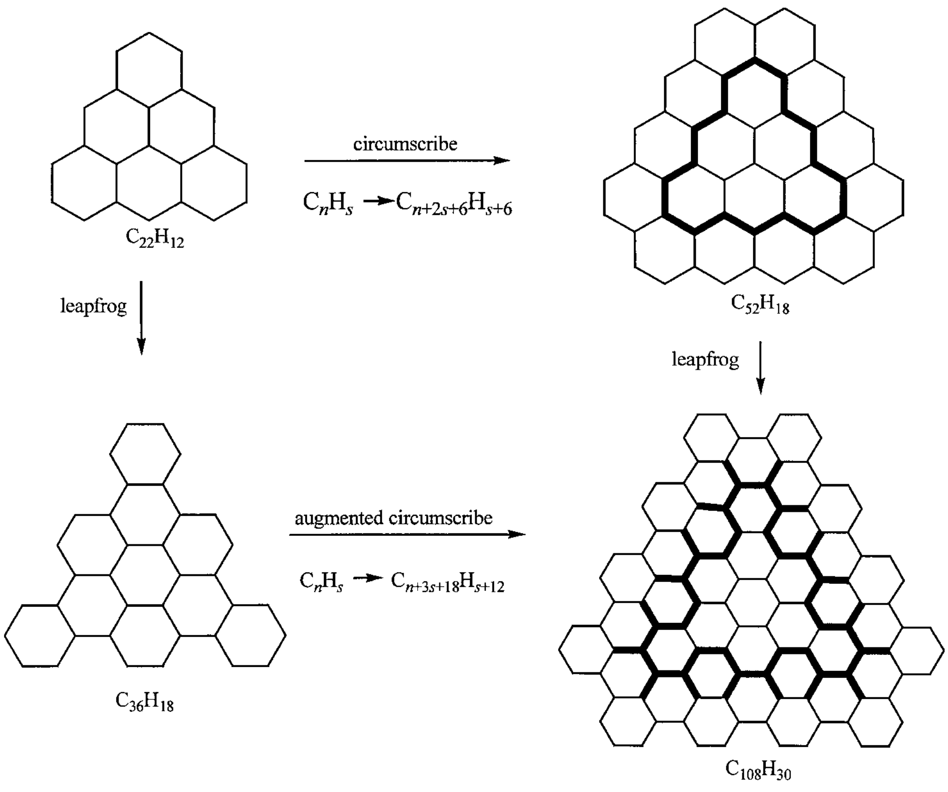
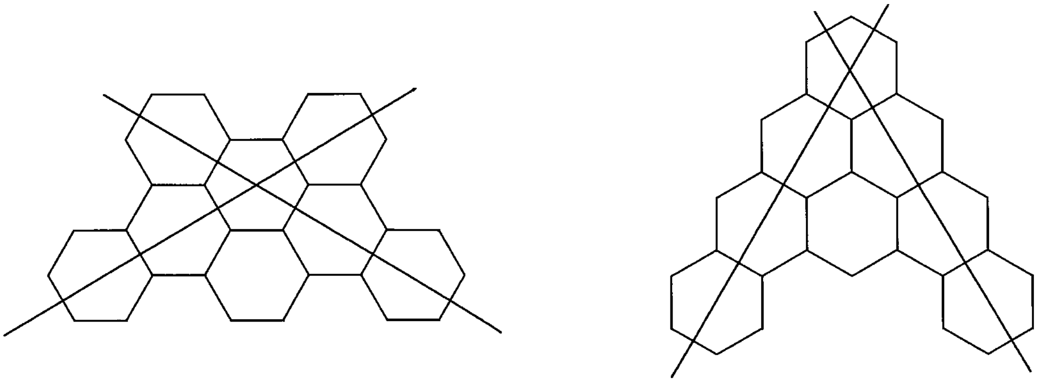


Figure 7. Comparison of circumscribing and leapfrog operations

constant-isomer series, the other polyradicals in Fig. 1 are only predecessors to their respective polyradical constant-one-isomer series. For example, circumscribing the $C_{33}H_{15}$ triradical once gives the $C_{69}H_{21}$ triradical, which is the first-generation member of the unique triradical D_{3h} constant-one-isomer series. The formula of $C_{69}H_{21}$ also corresponds to 12 more monoradical benzenoids that are the first-generation members of the monoradical constant-12-isomer series.[14] Similarly, circumscribing the $C_{46}H_{18}$ tetraradical twice gives the $C_{142}H_{30}$ tetraradical, which is the first-generation member of the unique formula of tetraradical D_{3h} constant-one-isomer series. The formula of $C_{142}H_{30}$ also corresponds to 46 diradical and 86 Kekuléan (nonradical) benzenoid hydrocarbons. The 46 $C_{142}H_{30}$ diradicals are the first-generation members of the diradical constant-46-isomer series, and the sum of $1 + 46 + 86 = 133$ is the total number of $C_{142}H_{30}$ benzenoid isomers belonging to the first generation of the constant-133-isomer series. Successively circumscribing the $C_{61}H_{21}$ pentaradical gives $C_{325}H_{45}$ as the first-generation member of the unique pentaradical D_{3h} constant-one-isomer series. The formula of $C_{325}H_{45}$ also corresponds 162 triradicals and 1471 monoradicals which are the first-generation members of the corresponding constant-isomer series.

While the isomer numbers and corresponding symmetry distribution of the benzenoid members for all the monoradical constant-isomer series match those of the benzenoid members of the diradical constant-isomer series, triradical constant-isomer series, tetraradical constant-isomer series, etc., the sum of the numbers for all radical degrees (including zero) of a given formula corresponds to the isomer number of the TRS constant-isomer series. Just like the leapfrog of the nonradical and diradical $C_{22}H_{12}$ benzenoids of the first generation of the constant-three-isomer series in Fig. 6 led to the $C_{36}H_{18}$ first-generation members of the TRS constant-three-isomer series, the leapfrog of the monoradical and triradical $C_{69}H_{21}$ first-generation members of the constant-13-isomer series leads to the corresponding $C_{150}H_{36}$ first-generation members of the TRS constant-13-isomer series. Similarly, the leapfrog of the nonradical, diradical and tetraradical $C_{142}H_{30}$ and the monoradical, triradical and pentaradical $C_{325}H_{45}$ first-generation benzenoid members of the constant-133-isomer and constant-1634-isomer series leads to the corresponding $C_{342}H_{54}$ and $C_{846}H_{84}$ first-generation members of the TRS constant-133-isomer and constant-1634-isomer series, respectively.

The above has reviewed the topological congruency that exists between the various benzenoid radical constant-isomer series and the TRS constant-isomer series. It is the equilateral triangular shape of the members of the polyradical series that imbued them with the unique properties responsible for their benchmark role in the discovery of the topological paradigm which characterizes the structures of benzenoid hydrocarbons.[7,14]



K = 45, E = 43.0652

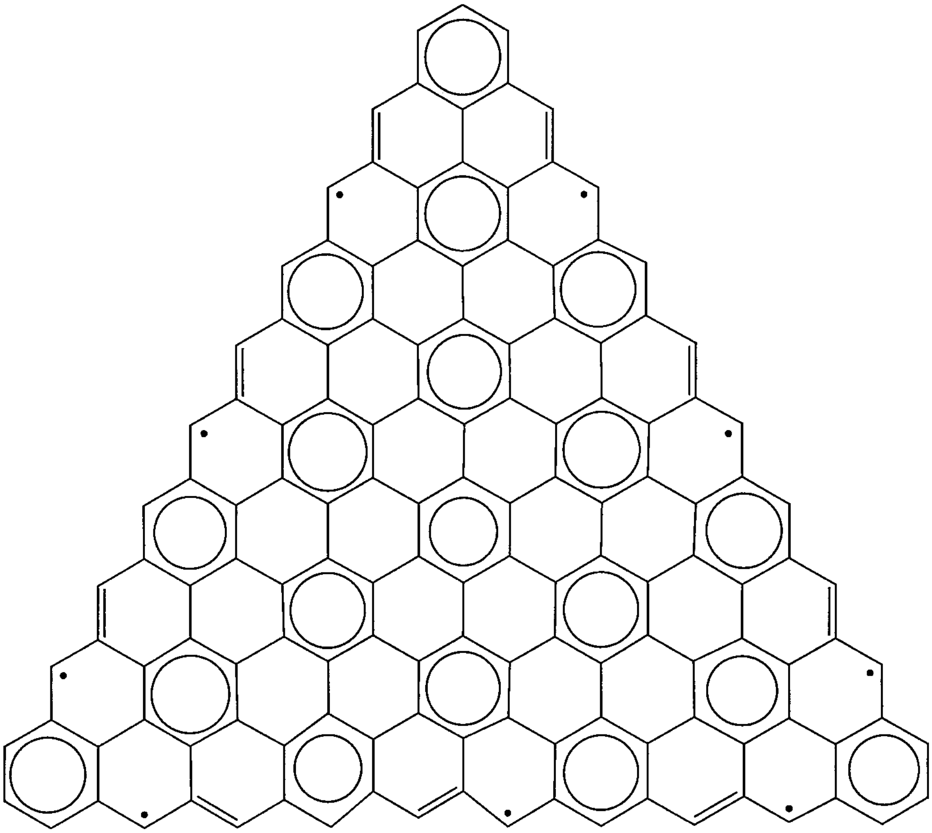
0.5029
0.6173
0.7562
1.0, 1.0, 1.0
1.2569
1.3691
1.4693
1.4845
1.8766
1.9569
2.1635
2.3892
2.6902

SC = 1 008, E = 40.8869

0, 0
0.6489
0.7992
1.0, 1.0, 1.0
1.2752
1.3789
1.41421
1.6041
1.8578
2.2681
2.3455
2.6703

Figure 8. The most and least stable $C_{30}H_{16}$ benzenoid isomers out 67 possible benzenoid isomers

In the comparison of the benzenoid triangular polyradicals in Fig. 1 with the associated leapfrog TRS in Fig. 2, symmetry was held constant. The smallest benzenoid formula having a set of isomers (67)[15] with both diradical (9) and TRS (1) benzenoid subsets is $C_{30}H_{16}$. The sole $C_{30}H_{16}$ TRS and a select diradical are given in Fig. 8 with their pπ-electronic energies (*E*) and HMO eigenvalue pairs listed beneath. These two isomers are worth comparing because they both have C_{2v} symmetry, two quarto perimeter regions (benzo appendages) and two selective lineations which are topological markers for fast recognition of the presence of ±1 eigenvalues. The TRS



$C_{141}H_{33}$

Figure 9. Maximum number of resonant sextets in the equilateral triangular nonaradical

has five resonant sextets, five bay perimeter regions and no solo perimeter regions and the diradical has four resonant sextets, two bay regions and five solo perimeter regions. The TRS is known but the diradical is not.[12] All the data in Fig. 8 are consistent with the chemistry and topology of these systems.

NUMBER OF CLAR RESONANT SEXTETS

The (maximum) number of resonant sextets in TRS benzenoid hydrocarbons (e.g. Fig. 2) is simply given by $N_c/6$. The maximum possible number of resonant sextets in the members of the triangular benzenoid polyradical series in Fig. 1 is given by the smallest integer to the following floor equation:

$$\text{max. No. of sextets} = \left\lfloor \frac{1}{2}\left(\frac{1}{3}t^2 + t + 2\right) \right\rfloor$$

The application of this equation can be illustrated by the triangular nonaradical with 55 rings in Fig. 9 which is the ninth-generation ($t = 9$) member, $\frac{1}{2}\left(\frac{1}{3} \times 81 + 9 + 2\right) = 19$. In the leapfrog of this nonaradical ($C_{141}H_{33} \rightarrow C_{330}H_{60}$), 19 resonant sextets goes to 330/6 = 55 resonant sextets.

CONCLUSION

Triangular benzenoid hydrocarbons have special properties which have numerous important ramafications ranging from understanding benzenoid reactivity and stability to organizing benzenoid structure–formula relationships. While the leapfrog algorithm in this comparative study held symmetry constant, the other topological parameters are systematically changed. Various descriptive topological generalizations are accumulated in the comparison of triangular polyradicals and their associated TRS benzenoids. Specifically, in the former, solo perimeter regions and electronic open shells which are maximized are characteristics of reactivity and, in the latter, bay perimeter regions and resonant sextets which are maximized are characteristics of stability.

The topological study of benzenoid hydrocarbons is important not only because of their prevalence but also because they are ideal model alternant PAHs. The study of ideal model alternant hydrocarbons provides the background for extensions of our understanding into nonalternant PAHs.

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