

Study of the origin of subspectrality in molecular graphs

Part II: Characteristic polynomials and eigenvalues of three series of related molecular graphs formed respectively from cyclobutadiene, benzene, and cyclooctatetraene

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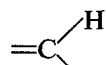
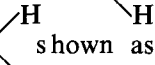
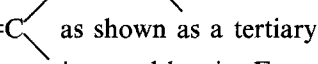
Summary. The subspectral origin of three families of molecules based on cyclobutadiene, benzene, and cyclooctatetraene is discussed. The graph theoretical decomposition of the fourfold cyclooctatetraene molecular graphs is presented in explicit form and has expedited the computation of their respective eigenvalues. The cyclic automorphism approach of Davidson is clarified and merged with the author's methodology leading to a more comprehensive procedure for rapidly determining the characteristic polynomial and eigenvalues of chemically significant molecular graphs. The graph theoretical determination of the characteristic polynomials and eigenvalues of two sixfold coronene-related molecular families is presented.

Key words: Characteristic polynomials — Eigenvalues — Subspectral — Cyclooctatetraene — Coronene — Cyclobutadiene

1. Introduction

Our previous work [1] traced the genesis of one type of subspectrality ultimately to precursor molecules of threefold or greater symmetry. Molecular graphs with a greater than twofold axis of symmetry possess a doubly degenerate eigenvalue subset [2]. Thus, deletion of a molecular vertex, replacement of a CH vertex by a heteroatom vertex, or replacement of H by a conjugated substituent leads to successor molecular graphs which still retain these eigenvalues once. Herein, another type subspectrality associated with three related families based on cyclobutadiene, benzene, and cyclooctatetraene is traced. Cyclobutadiene, benzene, and cyclooctatetraene all possess the eigenvalues of ± 2 , and all the eigenvalues of cyclobutadiene (0, 0, ± 2) are contained in cyclooctatetraene. It

will be shown that these three molecules are the first members of three related molecular series having twofold, threefold, and fourfold symmetry, respectively. Throughout this paper the carbon and hydrogen atoms and the $p\pi$ -bonds in all molecular graphs will be omitted and only the C-C σ -bond skeleton will be

shown. The various types of vertices referred to herein are methylene $=\text{C}$  shown as a primary (degree one) graph vertex, methine $=\text{C}$  shown as secondary (degree two) graph vertex, and carbon $=\text{C}$  as shown as a tertiary (degree three) graph vertex. Table 1 summarizes the notation used herein. For a comprehensive review about the importance of the characteristic polynomial, one should refer to the recent work of Trinajstić [3].

When two different conjugated polyene molecules have some common eigenvalues, they are said to be subspectral [2, 3]. Just as isomers are more similar than nonisomers and molecules with the same set of functional groups are more similar than molecules with different functional groups, subspectral molecules are more similar than molecules with no eigenvalues in common. Three subspectral families are formed from cyclobutadiene, benzene, and cyclooctatetraene. The members of the cyclobutadiene family have a twofold axis of symmetry, the benzene family members have threefold symmetry, and the members of the cyclooctatetraene family have a fourfold axis of symmetry. The origin of the subspectrality in these related families will be presented in this paper.

Table 1. Glossary of terms

a_4	Fourth coefficient in the characteristic polynomial
a_6	Sixth coefficient in the characteristic polynomial
α (α_c)	HMO Coulomb integral (of carbon)
α_3	No. of branches on a trigonal ring
α_4	No. of branches on a tetragonal ring
β	HMO exchange integral
d_i	No. of vertices of degree- i
$e(i, j)$	No. of edges with a vertex of degree- i at one end and a vertex of degree- j at the other end
e_k	An edge of weight k
ε	Energy level or HMO eigenvalue
E_π	Total $p\pi$ energy
G	A molecular or isoconjugate graph
G_x	A molecular graph with a single weighted vertex
G_k	A molecular graph with a single weighted edge
h	The weight of a heteroatom vertex [$h = (\alpha_x - \alpha_c)/\beta$]
k	The weight of an edge [$k = \beta_{cx}/\beta_{cc}$]
N (N_c)	No. of (carbon atom) vertices
$P(G; X)$	Characteristic polynomial of a molecular graph
q	No. of C-C σ -bond edges
r_n	No. of rings (cycles) of n vertices
v	Vertex
X	$(\varepsilon - \alpha)/\beta =$ graph eigenvalue
Z_k	Cycles containing edge k

While there is no doubt that 1,3-cyclobutadiene and 1,3,5,7-cyclooctatetraene possess strong similarities and have the common eigenvalues of $0, 0, \pm 2$, one might legitimately question their similarity to benzene which also has the eigenvalues of ± 2 . The absence of the zero eigenvalues in benzene makes it less similar to the hypothetical square cyclobutadiene and planar cyclooctatetraene molecules whose real chemistry is unknown, other than that they are antiaromatic while benzene is known to be aromatic. This latter dominant feature for these molecules should not be allowed to distract us from the qualitative thesis propounded in the prior paragraph suggesting that, other things being equal, subspectral molecules are expected to be more similar than molecules with no eigenvalues in common. Obviously, the magnitude of this subspectrality/similarity effect will be larger for molecules where the common eigenvalues include the frontier molecular orbitals (i.e., the HOMO and LUMO) which dominate their chemistry, and for molecules having a larger intersection of common eigenvalues. Also, the intervention of dominant specialized effects not directly governed by eigenvalues cannot be precluded and will have to be dealt with separately. Notable examples would include aromatic/antriaromatic, steric and size effects. Although, the concept of similarity is vague, it is nevertheless a useful descriptive means for comparing and visualizing chemical phenomena. The study of different ways of comparing molecules will eventually contribute to our better understanding of their chemistry. Herein, we have proposed one type or molecular similarity. The degree of overall influence of this proposed subspectral/similarity effect can only be determined after the factors which govern this phenomenon have been elucidated, and then it must be balanced against other effects.

Using cyclic automorphism subgroups, Davidson published a seminal paper on the spectral analysis of graphs [4]. The automorphism group of a molecular graph is the set of adjacency and edge-weight preserving isomorphisms of the structure. By associating graphs having cyclic automorphisms with symmetrical polymer networks composed of simpler monomeric substructural repeating units, it can be shown that the spectrum of eigenvalues of many molecular families devolves to the evaluation of a single monomer-derived irreducible subgraph with only one parameter (h). Thus, graphs with cyclic automorphism subgroups are regarded for purposes of spectral analysis as polymers or oligomers made up of fundamental monomeric building units (subgraphs). This approach also facilitates the recognition of molecular systems sharing a subspectrum of identical eigenvalues. Herein, we clarify and expand Davidson's approach while merging it with our graph theoretical methods.

The twofold symmetrical polyene molecules given in Fig. 1 have previously been studied experimentally or theoretically [5–8], and, heteroatom isoskeletal analogs of the pentagonal ring containing species in Figs. 1 and 2 are also known [9–11]. Study of the liquid crystal properties of derivatives of some of the related threefold molecules has been pursued [12–13]. Biphenylene (Fig. 1) and tetraphenylene (Fig. 2) were synthesized by CuCl_2 coupling of the dimagnesium Grignard of *o,o'*-dibromobiphenylene [14]. The tetraoxide of [2,3]tetranaphthylene (tetranaphthol[2,3]cyclooctatetrene, Fig. 2) has been characterized [15]. Bitropylyene is an isomer of anthracene/phenanthrene, and dibenzo[*b,h*]biphenylene

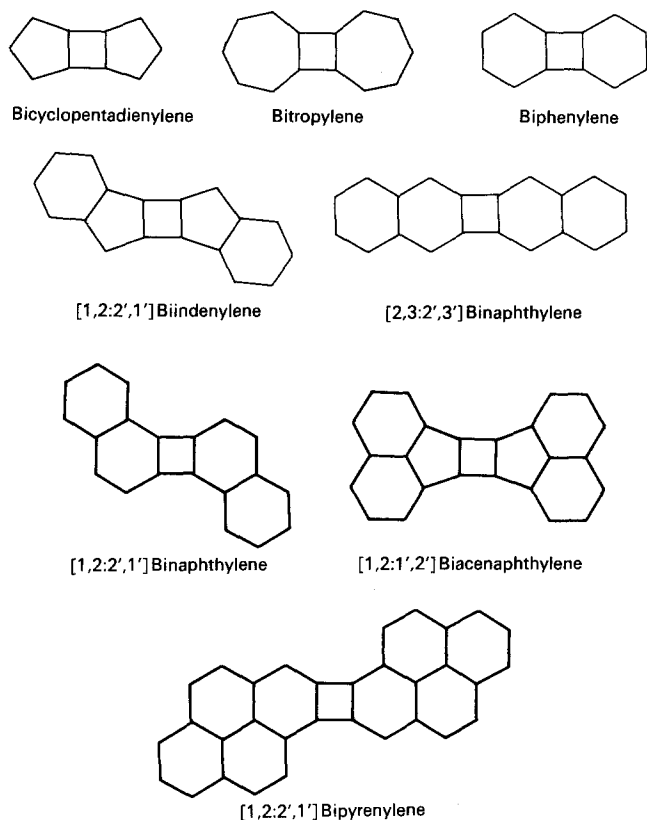
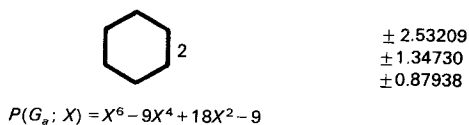


Fig. 1. Twofold molecular graphs of this study

([2,3:2',3']binaphthylene) and dibenzo[*a,g*]biphenylene ([1,2:2',1']binaphthylene), which are isomers of benzo[*a*]pyrene, have been synthesized [16, 17]. A close isomer of [1,2:2',1']bipyrenylene (Fig. 1) has been synthesized [18] and is of carcinogenic interest, as are the isomers of benzo[*a*]pyrene.

2. Common fragment subgraphs with edge weight of two

In the decomposition of threefold ring centric molecular graphs, one obtains a fragment subgraph with an edge of weight two [1]. This same fragment is also obtained from twofold ring centric molecular graphs in which the central ring is four membered [3]. Thus, triphenylene and biphenylene both have the following fragment subgraph and associated eigenvalues:



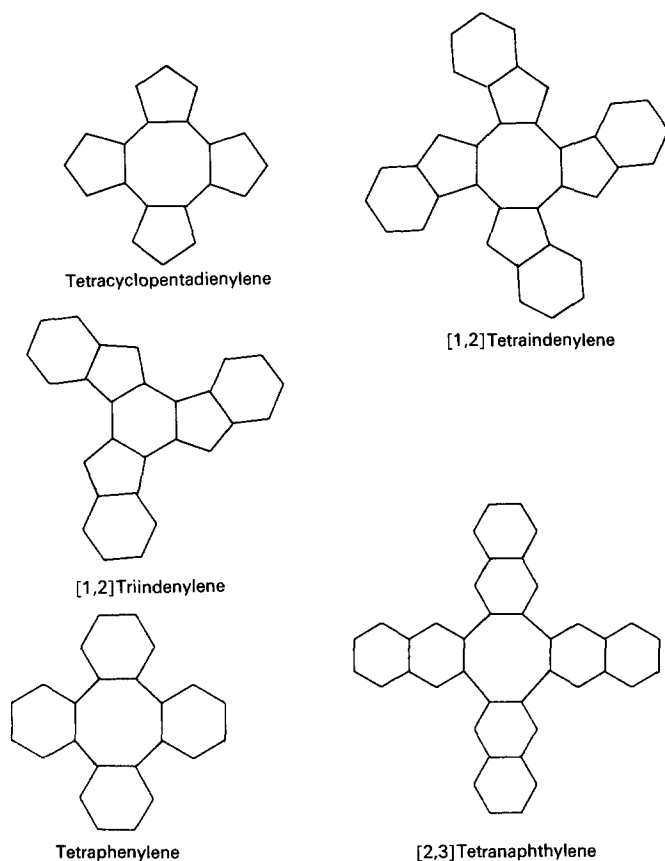
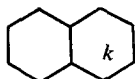


Fig. 2. Some threefold and fourfold molecular graphs of this study

Since the eigenvalues of biphenylene are present in tetraphenylene, the above subgraph and L_6 are also components of tetraphenylene.

From Fig. 3, it is apparent that [1,2:2',1']binaphthylene is subspectral to [1,2]tetranaphthylene, and the two molecular graphs with greater than twofold symmetry have doubly degenerate subsets. All three molecular graphs in Fig. 3 have the same subspectral component. While only the first two molecules have been synthesized [19], an isomeric derivative of the latter has been prepared [15], and there is considerable interest in these molecular systems. For example, C_{60} buckminsterfullerene can be formed by fusing the three cove regions in tribenzo[*a,g,m*]triphenylene (Fig. 3) and then fusing the resulting bowl-shaped species together [20].

The rules for factorization of [1,2;2',1']binaphthylene into irreducible subgraphs G_+ and G_- , where G_+ has and edge weight of 2, has been described by D'Amato [21]. It is only worthwhile noticing that application of Eq. (5) in Table 2 for the single parameter of $k = 0$ and 2 on the following general subgraph gives the characteristic polynomials for both G_- and G_+ , respectively.



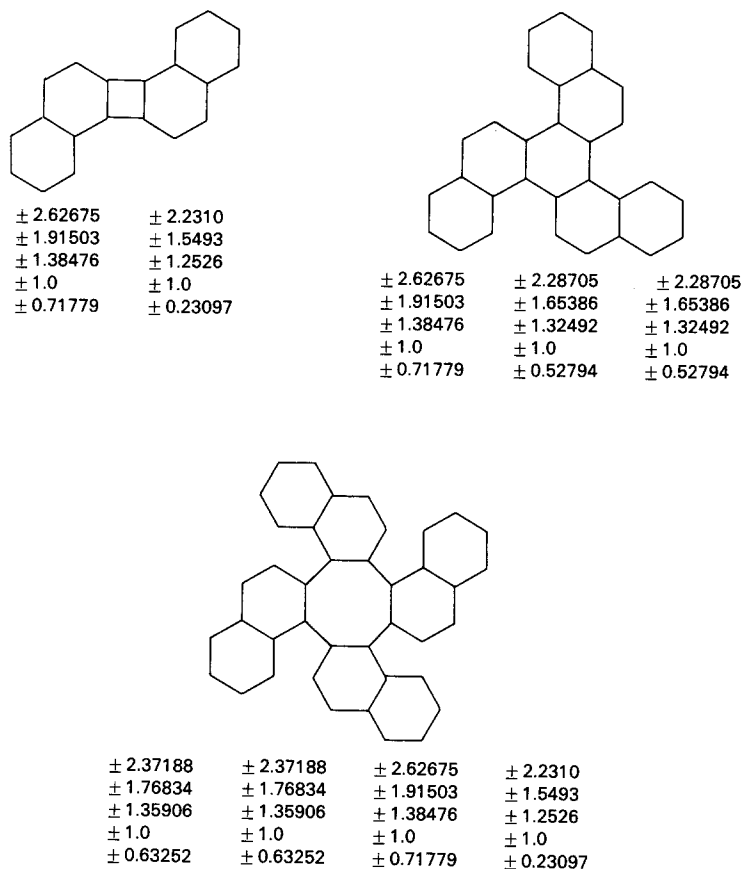


Fig. 3. Subspectrally related to molecular graphs

Figure 4 summarizes all the G_+ and G_- subgraphs and their characteristic polynomials and eigenvalues for common twofold cyclobutadiene ring centric graphs examined in this study. In addition, it should be noted that all the G_+ subgraphs in Fig. 4 also appear in the threefold ring centric molecular graphs previously published [1, 8].

Symmetrical molecular graphs that can be decomposed by mirror plane fragmentation to give a right fragment with threefold (or greater) symmetry will possess the doubly degenerate eigenvalue subset and nondegenerate eigenvalues associated with the threefold fragment. Molecular graphs possessing a twofold axis of symmetry at the center of a hexagonal ring flanked by two identical threefold subgraphs will possess the doubly degenerate eigenvalue subset associated with the threefold subgraphs. Tetrabenz[*a,c,l,n*]pentacene has both a mirror plane of symmetry and a twofold axis and has the eigenvalues of triphenylene. Diphenanthro[9,10-*a*:9',10'-*h*]anthracene has only a twofold axis of symmetry and only has the doubly degenerate eigenvalues of triphenylene.

Table 2. Equations for calculation of characteristic polynomials of molecular graphs

Equation number

-
- (1) $a_4 = \frac{1}{2}(q^2 - 9q + 6N_c) - 2r_4 - d_1 - d_4 - 3d_5 - 6d_6 - \dots$
- (2) $a_6 = -\frac{1}{6}(q^3 - 27q^2 + 116q) - N_c(3q - 16) - 2r_6 - e(3, 3) + (q - 6)e(2, 1) + (q - 5)e(3, 1) + 2(q - 4 - \alpha_4)r_4 + r_3$
- (3) $P(G; X) = X^N - qX^{N-2} - 2r_3X^{N-3} + a_4X^{N-4} - [2r_5 - 2(q - 3 - \alpha_3)r_3]X^{N-5} + a_6X^{N-6} + \dots$
- (4) $P(G_x; X) = XP(G_x - v_x; X) - hP(G_x - v_x; X) - k^2[XP(G_x - v_x; X) - P(G; X)]$
for edge/vertex weighted graphs
- (5) $P(G_k; X) = P(G_k - e_k; X) - k^2P(G_k - (e_k); X) - 2k \sum P(G_k - Z_k; X)$
for edge weighted graphs
- (6) $P(G_0; X) = P(G; X) + P(G_0 - v_0; X)$ for right mirror-plane fragments
- (7) $P(G_{e1}; X) = P(G_{e1} - e_\omega; X) - P(G_{e1} - (e_\omega); X) + \sum P(G_{e1} - Z_\omega; X)$
for the identical fragments of vertex-centric threefold graphs
- (8) $P(G_{e2}; X) = P(G_{e2} - e_\omega; X) - P(G_{e2} - (e_\omega); X) - \sum P(G_{e2} - Z_\omega; X)$
for the identical fragments of ring-centric threefold graphs
- (9) $P(G_{4j}; X) = P(G; X) - P(G - (e); X)$
for identical fragments of ring-centric fourfold graphs
- (10) $P(G_1; X) = P(G_1 - e_1; X) - P(G_1 - (e_1); X) - h \sum P(G_1 - Z_1; X)$
for the generalized irreducible unit subgraph of ring-centric sixfold graphs with $h = \pm 1, \pm 1, \pm 2$
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3. Factorization of fourfold molecular graphs

Figure 5 illustrates the decomposition of the fourfold cyclooctatetraene ring centric graph from Fig. 3; Davidson presented this decomposition scheme in more abstract form [4]. Here our contribution is the recognition that the characteristic polynomial of the (fourfold fragment, 4/) subgraph G_{4j} is given by $P(G_{4j}; X) = P(G; X) - P(G - (e); X)$ where G is its isoconjugate analog graph and $G - (e)$ is obtained by deleting the corresponding edge e and its associated vertices from G . Figure 6 summarizes all the G_{4j} subgraphs of this study along with their characteristic polynomials and eigenvalues.

Whenever a smaller bipartite graph can be embedded onto a larger one, then the latter will possess the eigenvalues of the former [22]. In Fig. 4, various nonedge-weighted molecular graphs are embeddable by methyl, ethene, allyl, and pentadienyl, giving eigenvalues of 0, ± 1 , $\pm \sqrt{2}$, and ± 1 and $\pm \sqrt{3}$, respectively.

These embeddings were used as a cross-check for the computations presented in Figs. 4 and 6. Both 2-methylenylpentadienyl and 1,8-dimethylenyl-naphthalene have two distinct methyl embeddings and are doubly degenerate in eigenvalues of zero. Both L_7 and benzyl have one distinct methyl embedding and one zero eigenvalue. The molecular graphs of L_5 , benzyl, 1-methylenyl-2-(1'-allyl)benzene, 1,8-dimethylenyl-naphthalene, 1-methylenyl-2-(1'-allyl)naphthalene, 1,2-divinyl-naphthalene, and 1-methylenyl-9-vinylphenaleny are embeddable by ethene and have eigenvalues of ± 1.0 . Many of the 2-edge weighted molecular graphs (Fig. 4) and their complex-edge weighted analogs (Fig. 6) were simultaneously embeddable by ethene and have eigenvalues of ± 1.0 . The molecular graphs of L_7 and 1-methylenyl-2-vinylbenzene were embeddable one way and 1,2-divinylbenzene and 1-methylenyl-2-(1'-allyl)naphthalene were embeddable two ways by allyl and had the corresponding number of eigenvalues of $\pm\sqrt{2}$. 1,8-Dimethylenyl-naphthalene was embeddable by pentadienyl and has $\varepsilon = \pm 1.0$ and $\pm\sqrt{3}$.

4. Factorization of sixfold coronene-related molecular graphs

The decomposition of threefold coronene-related molecular graphs has been presented [23]. Herein, the factorization of two types of sixfold coronene-related molecular graphs will be detailed as per Davidson's method [4]. Davidson used cyclic automorphism subgroups to factorize coronene into a generalized irreducible unit subgraph with a single parameter for the purpose of obtaining all the

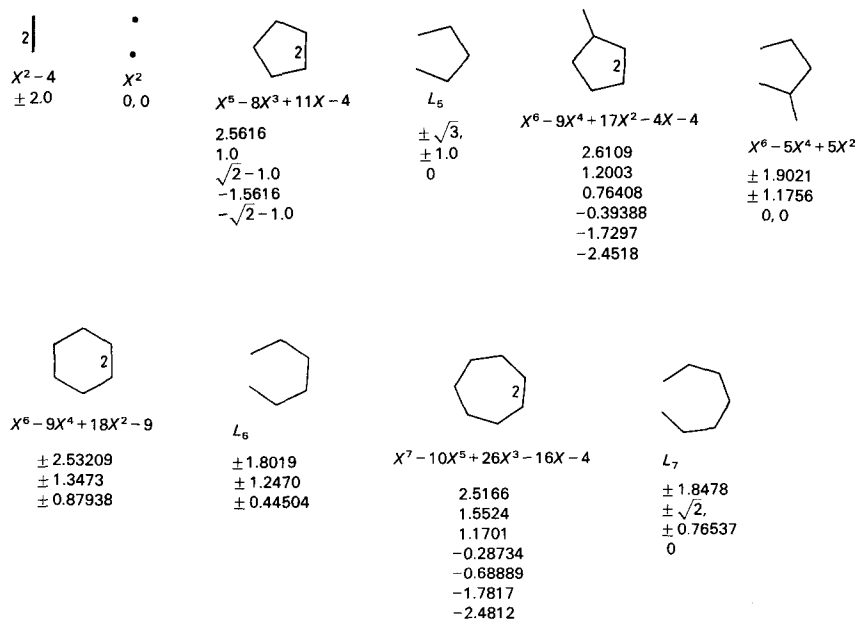


Fig. 4. Fragment subgraphs of related twofold and fourfold molecular graphs

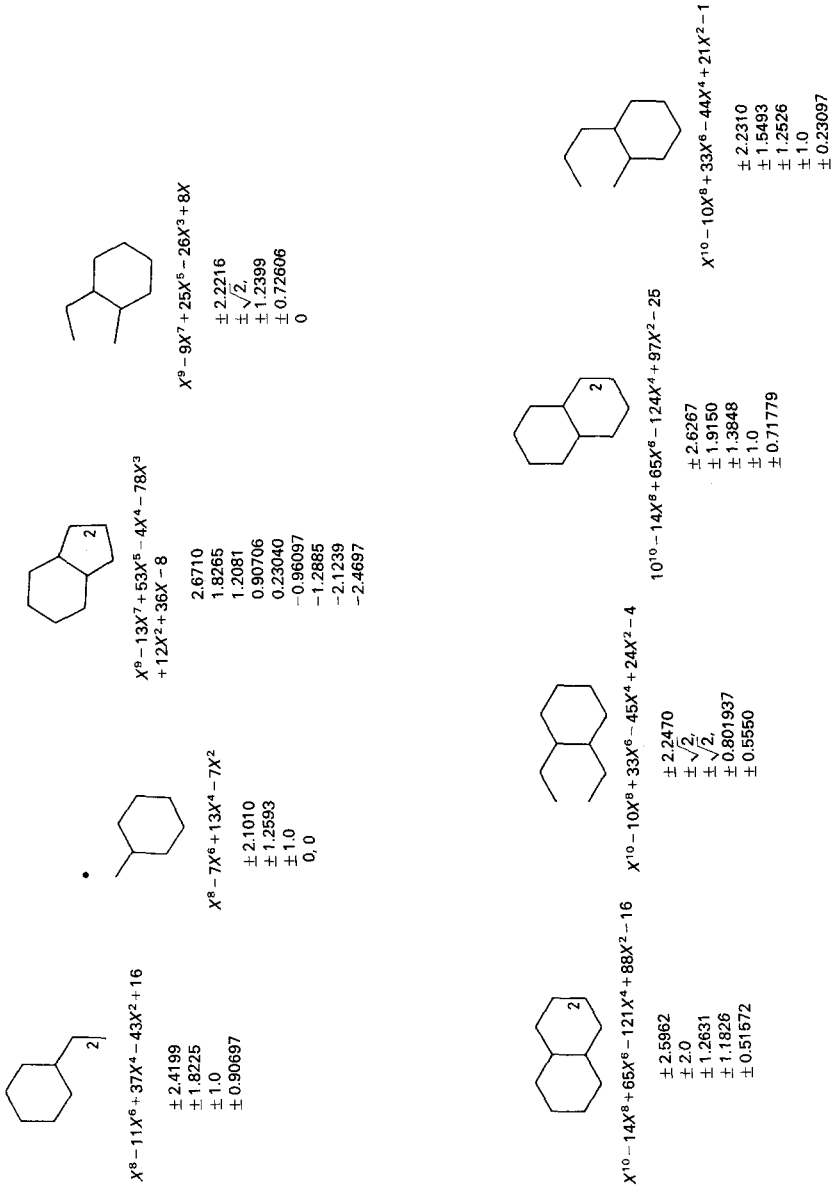


Fig. 4. (continued)

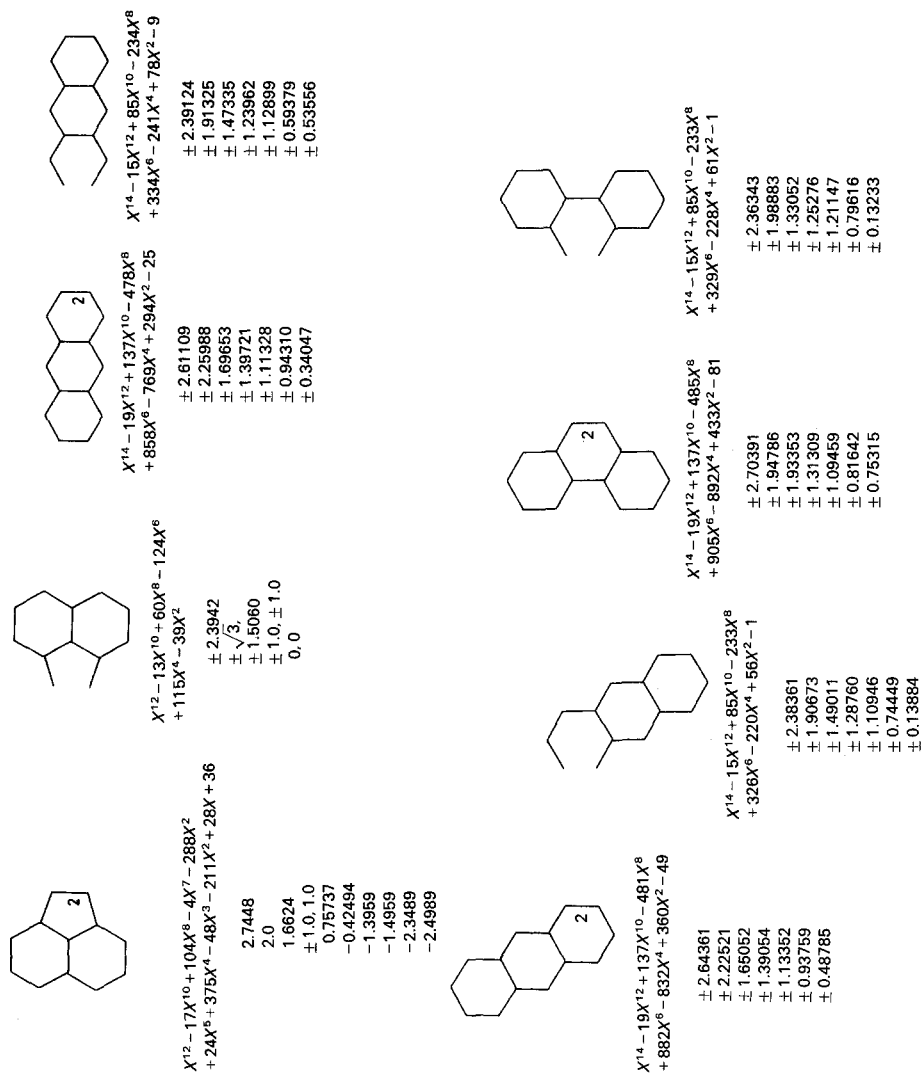


Fig. 4. (continued)

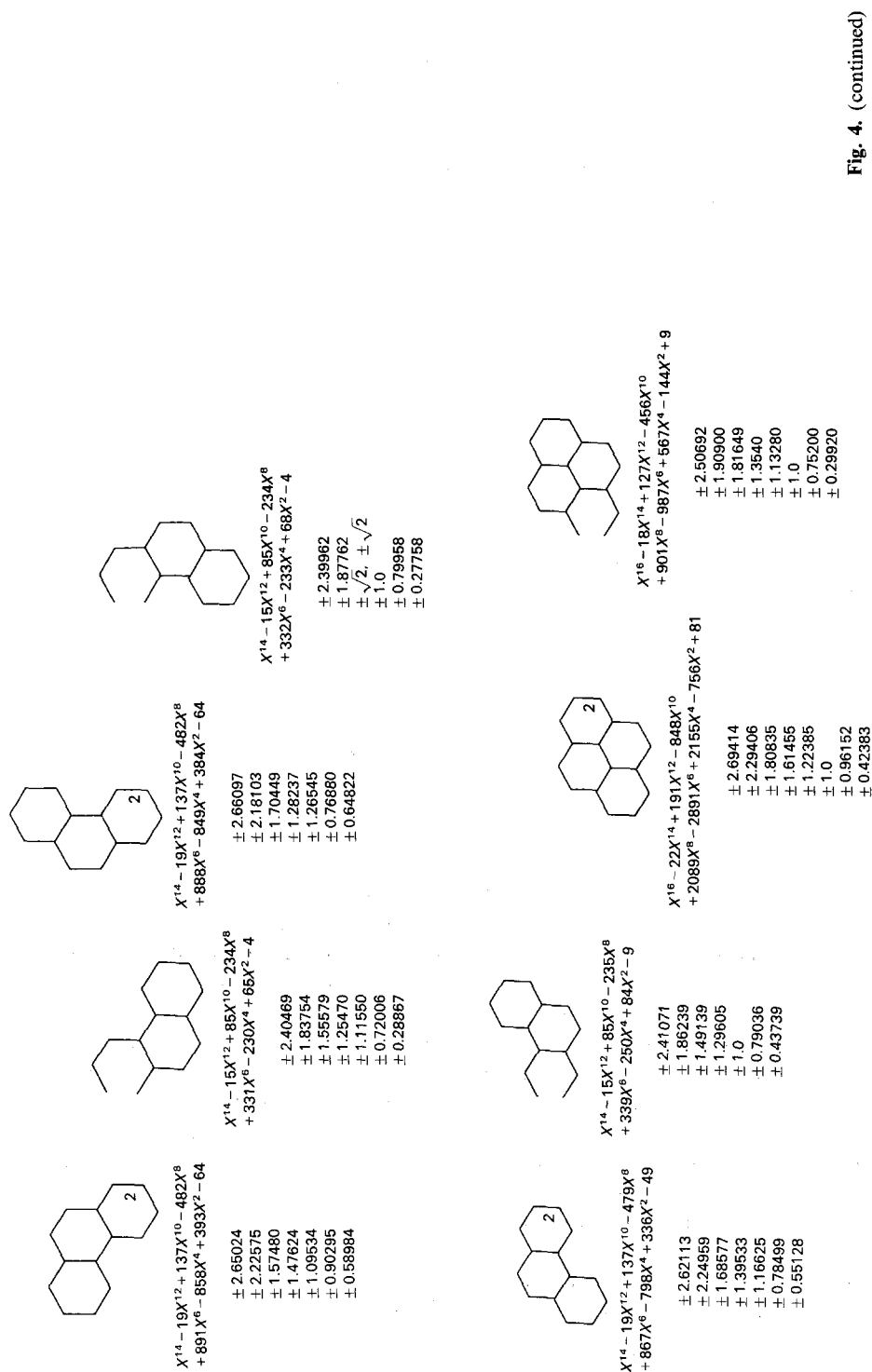
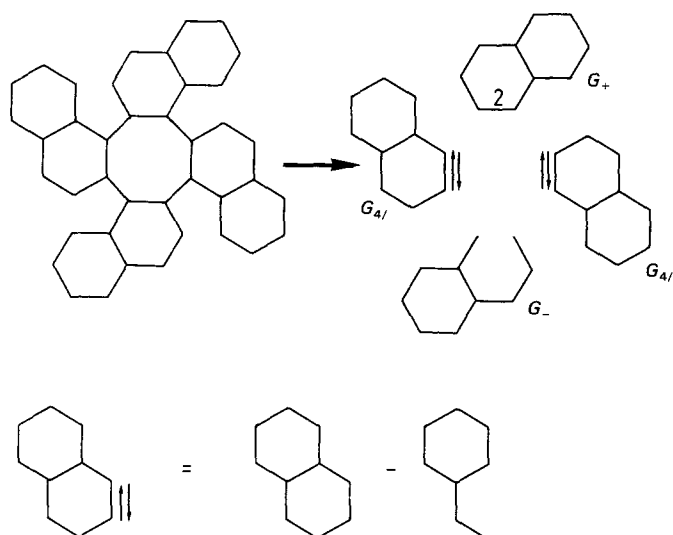


Fig. 4. (continued)



$$\begin{aligned}
 P(G_{A_i}; X) &= P(\text{naphthalene}; X) - P(\text{styrene}; X) \\
 &= (X^{10} - 11X^8 + 41X^6 - 65X^4 + 43X^2 - 9) - (X^6 - 8X^4 + 19X^2 - 16X^2 + 4) \\
 &= X^{10} - 12X^8 + 49X^6 - 84X^4 + 59X^2 - 13
 \end{aligned}$$

$$\pm 0.63252$$

$$\pm 1.0$$

$$\pm 1.35906$$

$$\pm 1.76835$$

$$\pm 2.37188$$

Fig. 5. Decomposition of [1,2]tetranaphthylene into fragment subgraphs

eigenvalues for coronene. However, his method was not made explicit and he used symbolic and notational devices which were detailed in manuscripts submitted (references 1–3) [4] but apparently never published. Figure 7 gives two general coronene-related series and their corresponding irreducible unit subgraphs. Here G_i represents pendant fragment subgraphs that do not destroy the sixfold symmetry associated with coronene and $h = \pm 1, \pm 1$, and ± 2 . Since these molecular graphs have a doubly degenerate eigenvalue subset given by $h = \pm 1$, if G_i is a bipartite subgraph (i.e., corresponds to an alternant hydrocarbon) then obtaining all the eigenvalues for these molecular graphs reduces to obtaining the eigenvalues of the irreducible unit subgraph for $h = 1$ and 2. By the pairing theorem and the double degeneracy, the remaining eigenvalues are simply written down from those obtained. This leads to substantial reduction in effort, since we have shown how to obtain the characteristic polynomial of small to moderate sized molecular graphs rapidly by using the equations in Table 2. This approach will now be illustrated by solving the eigenvalues for hexabenzozo[*a,d,g,j,m,p*]coronene and hexabenzozo[*bc,ef,hi,kl,no,qr*]coronene, which have been obtained previously [8].

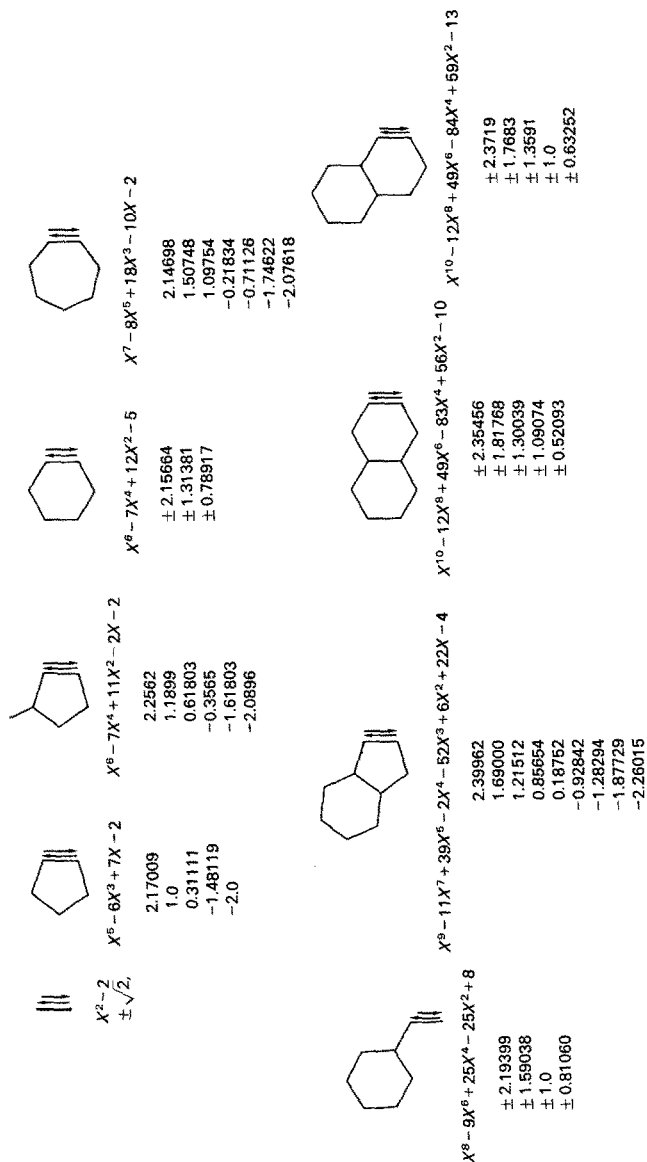


Fig. 6. Complex-edge fragment subgraphs of fourfold molecular graphs

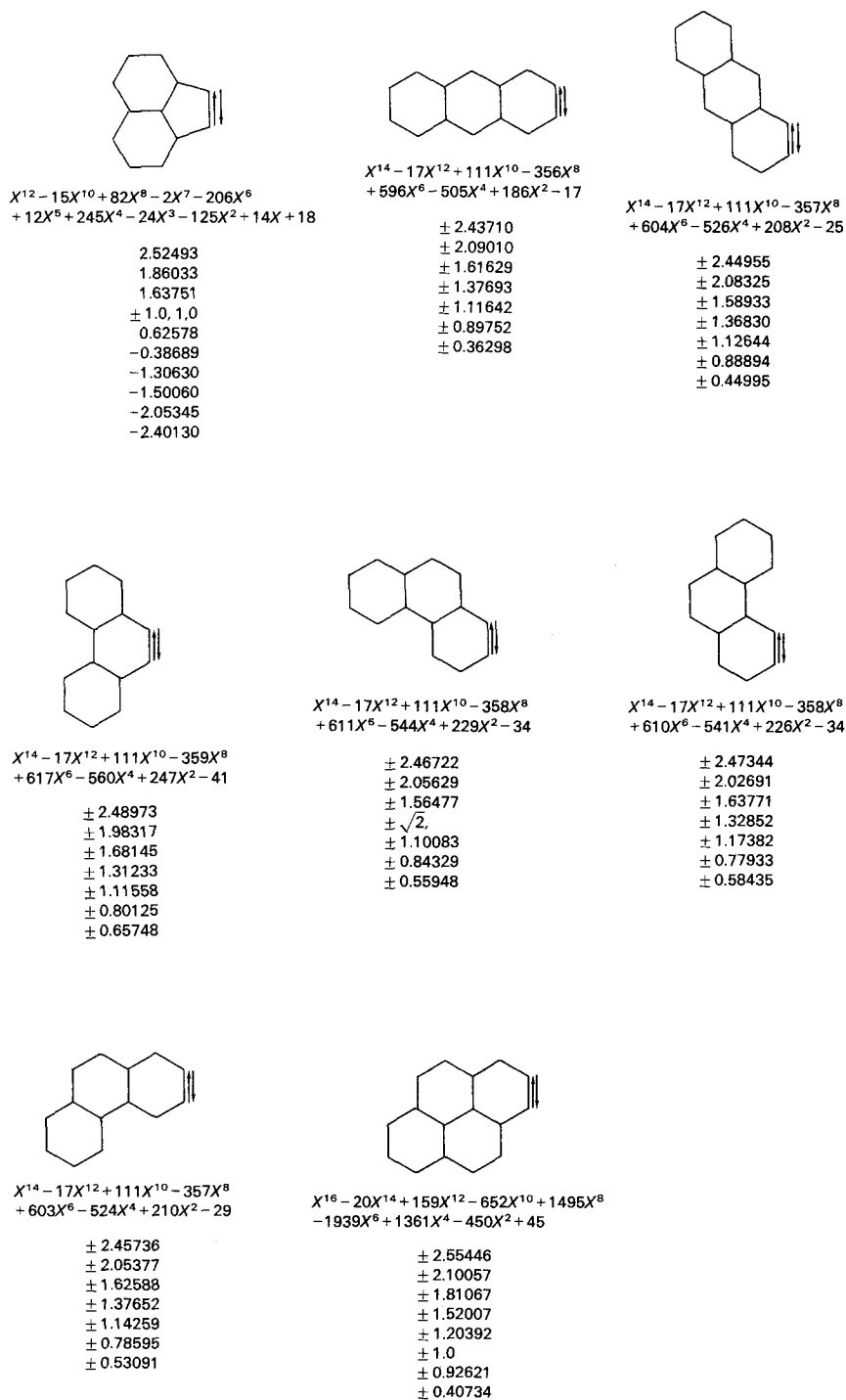


Fig. 6 (continued)

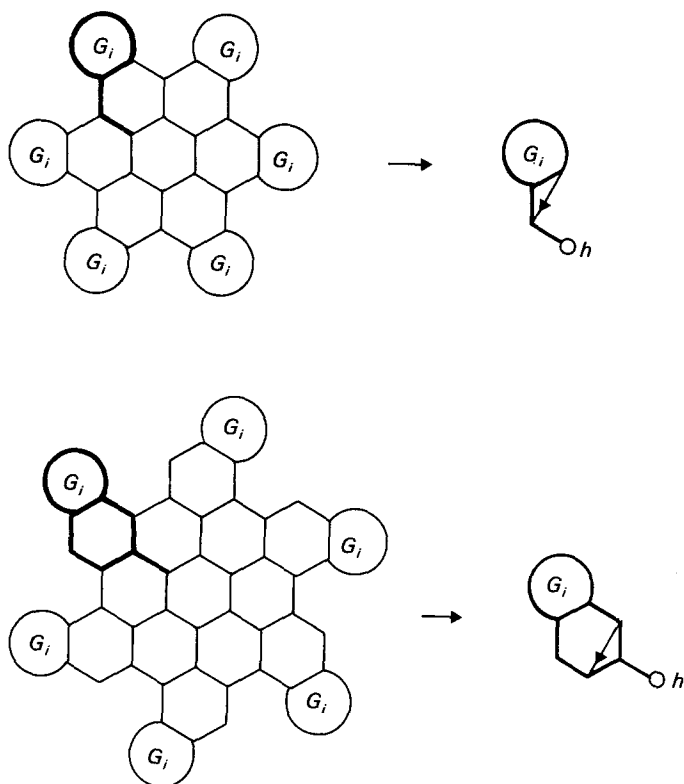


Fig. 7. Factorization of sixfold coronene-related molecular graphs into generalized irreducible unit subgraphs where $h = \pm 1, \pm 1, \pm 2$

Figure 8 illustrates how hexabenzocoronene can be decomposed into six subgraphs with weighted vertices of $h = \pm 1, \pm 1, \text{ and } \pm 2$, and which can be generalized to one irreducible unit subgraph with the parameter h . Using Eq. (4) in Table 2, this irreducible unit subgraph is converted into two subgraphs without a weighted vertex. To obtain the characteristic polynomial of these resulting subgraphs the following relation will be needed:

$$P(G_1; X) = P(G_1 - e_1; X) - P(G_1 - (e_1); X) - h \sum P(G_1 - Z_1; X)$$

where $G_1 - e_1$ is the subgraph obtained by deleting the complex edge e_1 from G_1 , $G_1 - (e_1)$ is the subgraph obtained by deleting the complex edge with its vertices, $G_1 - Z_1$ is the subgraph obtained by deleting the cycle Z_1 containing the complex edge, and $h = \pm 1, \pm 1, \text{ and } \pm 2$. Consider the generalized irreducible unit subgraph (G_6), of hexabenzocoronene. Application of Eq. (4) eliminates the weighted vertex h to give the two complex edge weighted graphs

shown in Fig. 8, which then are transformed via the above equation to give the polynomial shown. Solving this polynomial for $h = -1$ and -2 gives two different polynomials that lead to the eigenvalues shown, and which can be completed by using the pairing theorem and the degeneracy for $h = \pm 1$. These results agree with the eigenvalues previously obtained by another method [1, 8].

A further example is provided by the following characteristic polynomial/eigenvalue solution for hexabenzobenzene using its irreducible unit subgraph (Fig. 7). Using Eq. (4) in Table 2 followed by the application of the above equations results in

$$\begin{aligned}
 & \text{Diagram 1} = \text{Diagram 2} - h \text{Diagram 3} = \\
 & \text{Diagram 4} - \text{Diagram 5} - h \left(\text{Diagram 6} + \text{Diagram 7} \right) \\
 & -h \left(\text{Diagram 8} - \text{Diagram 9} - h \left(\text{Diagram 10} + \text{Diagram 11} \right) \right) \\
 & = X^7 - 7X^5 + 13X^3 - 7X - (X^5 - 3X^3 + 2X) - h[(X^2 - 1) + X^6 - 6X^4 + 9X^2 - 4] + h^2(X^3 - X) \\
 & = X^7 - 8X^5 + 16X^3 - 9X - h(X^6 - 6X^4 + 10X^2 - 5) + h^2(X^3 - X).
 \end{aligned}$$

Solution of this latter polynomial gives the following eigenvalues which are in complete agreement with previous results [1, 8]:

$h = 1$	$h = 2$
0.46477	0.61803
± 1.0	± 1.0
-1.34807	-1.61803
1.51484	-1.79129
-2.11838	2.0
2.48685	2.79129

In passing, it should be noted that hexabenzobenzene can be embedded three distinct ways by ethene and two distinct ways by benzene leading to seven eigenvalue pairs of ± 1.0 and two eigenvalue pairs of ± 2.0 . Likewise,

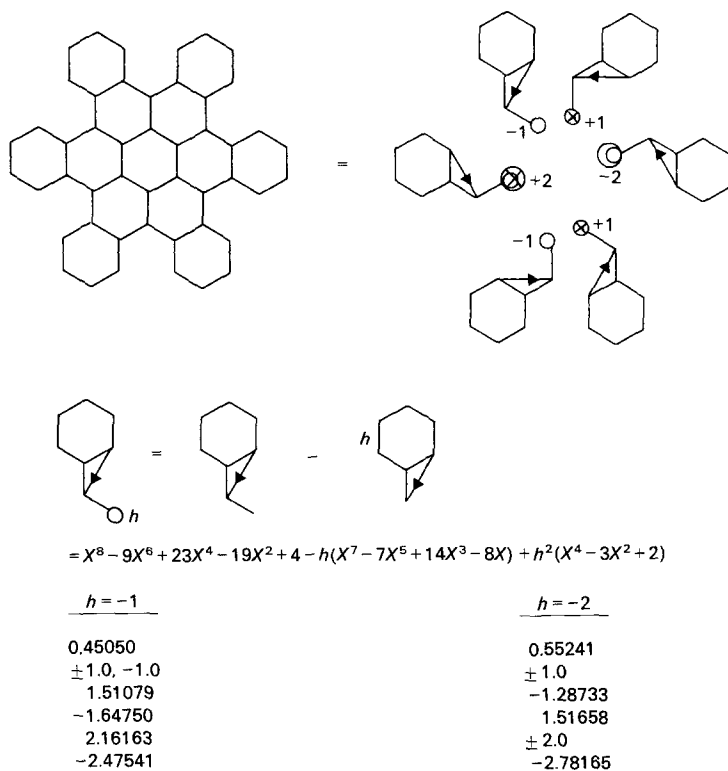


Fig. 8. Factorization of hexabenzo[*a,d,g,j,m,p*]coronene into irreducible subgraphs

hexabenzo[*bc,ef,hi,kl,no,qr*]coronene can be embedded by ethene in six distinct ways and by 1,3-butadiene in one way leading to six eigenvalue pairs of ± 1.0 and eigenvalues of $\pm \frac{1}{2}(\sqrt{5} \pm 1)$; these results are consistent with the computed results. Figure 9 summarizes the results for hexa[2,3]naphtho[*a,d,g,j,m,p*]coronene which can be embedded by naphthalene, and by allyl in six different ways, four of them being mutually exclusive. In general, for the first coronene-related family in Fig. 7, embedding by the pendant G_i subgraph is always possible if the molecular graph also has six twofold axes of rotation (as do coronene, hexabenzo[*a,d,g,j,m,p*]coronene, and hexa[2,3]naphtho[*a,d,g,j,m,p*]coronene).

5. Conclusion

The origin of subspectrality in chemically relevant molecular graphs has been determined. The approach of Davidson has been clarified and merged with the author's methodology for rapidly determining the characteristic polynomial of molecular graphs without the aid of group theory. This work contributes toward the comprehensive application of graph theory in the determination of the

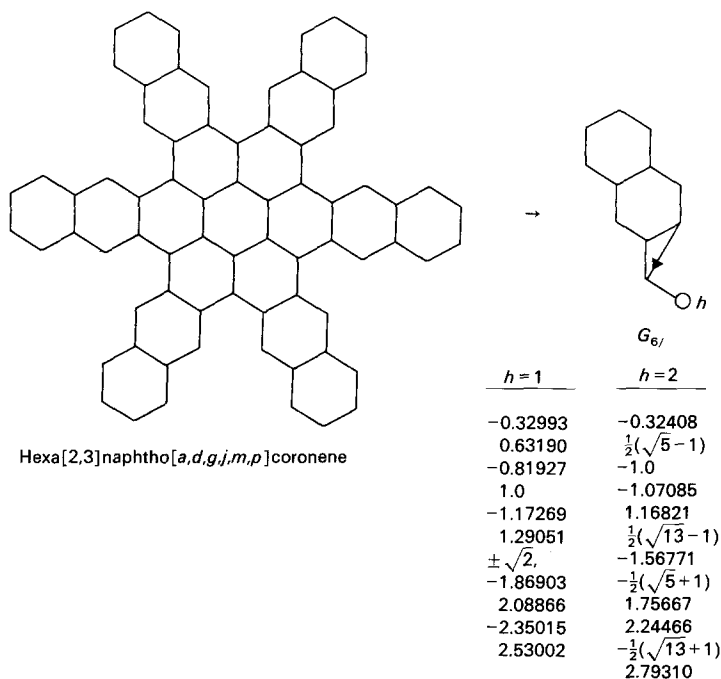


Fig. 9. Eigenvalue solution of hexa[2,3]naphtho[a,d,g,j,m,p]coronene

characteristic polynomials and eigenvalues of molecules. The fourfold and sixfold molecular graphs of this work possess doubly degenerate eigenvalue subsets. Deletion of a vertex, substitution of a heteroatom at any vertex, or placement of a polyene substituent at any position on these molecular graphs leads to successor molecular graphs still possessing the doubly degenerate eigenvalues of these fourfold or sixfold precursors once. Thus, the eigenvalues presented in this paper represent a compact compendium of select eigenvalues for many more molecules than those presented in Figs. 1–3, 8 and 9.

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