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On Endospectral Bipartite Graphs

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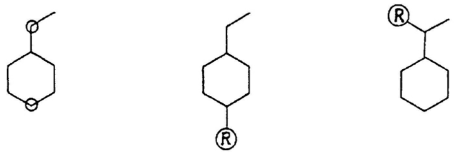
A novel approach is proposed to determining and constructing endospectral bipartite graphs. More than fifty new species and families of hexagonal lattice with endospectral pairs are listed and principles of their generation are outlined.

INTRODUCTION

Isospectral graphs are nonisomorphic graphs having the same sequence of eigenvalues. The importance of isospectrality is relevant to the inverse problem[1] emerging in science and technology which also plays a vital role in some special fields.[2,3] In studying the normal vibration of a membrane, Kac[4] raised the question: »Can one hear the shape of a drum?«, that is, can one determine the shape of a vibrating membrane or »drum skin« from the spectrum of its characteristic frequencies?[5] The answer was found to be negative for the high-dimensional torus.[6–8] Recently, Cipra[8] pointed out that »everyone marches to the beat of a different drummer, but all the drums sound the same«. Quite similar in chemistry, different molecules can have identical spectra[10–21] for the Hückel Hamiltonian, thus the characteristic polynomial would not uniquely characterize a structure.[22–25] Nevertheless, the study of isospectrality of graphs may renew the contents of characteristic polynomials,[19–26] giving an insight into the »inverse problem« from the spectra to the molecular structures.

The endospectral graphs are characterized by the presence of a pair of endospectral points, that is, the linking of a fragment to one of the two points will result in a pair of isospectral graphs. A well-known example is the styrene graph displayed in Figure 1, where endospectral points are marked with small circles. When radical R attaches to either of the two endospectral points, the isospectral pair, 1a and 1b, is produced.[26,28]

There hase been a continuous interest in investigating this kind of graphs,[26–41] and much progress on endospectral trees has been made by Knop and coworkers.[38] They tabulated such graphs exhaustively up to sixteen vertices with the valency of four or less. More recently, Randić and coworkers[26] revisited this topic with the emphasis on cyclic graphs. They exhibited new species of polyhex with pending bonds that are endospectral and pointed out that not much was known about the construction of such graphs.



1 1a 1b

Figure 1. Endospectral graph 1: styrene and the derived isospectral pair 1a and 1b.

As polyhexes are bipartite and exist widely, they are worth dealing with again in this paper. We have used the partition technique to transform the characteristic polynomial of the graph into the following product[34]

$$P_G(x) = P_B(x)\, P_{C'}(x) \tag{1}$$

where G symbolizes the graph, B and C represent subgraphs of G obtained by erasing all edges connecting B and C. Graph C' is derived from C by adjusting some weights of vertices and edges in accordance to Ref. 34. Since C' is smaller than G, but offers as much information as G, it can be called the contracted graph of G. The following statement is true:[34] if endospectral graph G is contracted without eliminating its endospectral points, then C' is also endospectral with endospectral points invariant. The inverse of this statement is also valid, *i.e.* C' can couple with B to give G with endospectral points unchanged.

If G is bipartite, B can be a collection of vertices of equal parity, then C' consists of all the remaining vertices of opposite parity and Eq. (1) behaves similarly to the 'wrapping' procedure,[31,32] which we will employ in this paper to treat such polyhex graphs with endospectral points of equal or different parity. Starting from some known results,[26–40] we will proceed to present numerous novel species. Various families of hexagonal lattice with endospectral pairs are listed and principles of their generation are outlined.

THEORETICAL BACKGROUND

As it is known, the vertices of a bipartite graph can be classified acording to their parity so that the first neighbors of each vertex are all of the opposite parity. Let G have N vertices, n be the number of the odd-parity vertices, and m $(= N-n)$ be the number of even-parity ones and satisfy $n \leq m$. One can label the odd vertices from 1 to n and the even ones from n+1 to N thus, the two collections of vertices are

$$\begin{aligned} V^-(G) &= \{\mu\} \qquad 1 \leq \mu \leq n \\ V^+(G) &= \{\nu\} \qquad n+1 \leq \nu \leq N \end{aligned} \tag{2}$$

Obviously, in bipartite graphs, all edges are incident to a pair of vertices of different parity, so the adjacency matrix of G is reduced into the following form

$$A = \begin{bmatrix} 0^- & B \\ B' & 0^+ \end{bmatrix} \tag{3}$$

where 0^- and 0^+ are null-blocks of the order n and m, respectively, and $\boldsymbol{B}$ (whose entry b_{ij} equals 1 if there is an edge between the vertices i and j, and 0 otherwise) is a submatrix of $n \times m$ while $\boldsymbol{B'}$ is the transpose of $\boldsymbol{B}$. The sequence of eigenvalues and the components (coefficients) of eigenvectors can be denoted as

$$\begin{aligned} X(G) &= \{x_i\} \qquad && 1 \le i \le N \\ C(G, x_i) &= \{c_\sigma(G, x_i)\} \qquad && 1 \le \sigma \le N \end{aligned} \tag{4}$$

According ot Eq. (3), the square of the adjacency matrix of G will be

$$A^2 = \begin{bmatrix} BB' & 0 \\ 0' & B'B \end{bmatrix} \tag{5}$$

where $\boldsymbol{BB'}$ and $\boldsymbol{B'B}$ are square blocks of the order n and m, 0 and 0' representing null matrices. Eq. (5) means that, if one regards $\boldsymbol{A}^2$ as the adjacency matrix of graph L, then L will be a disconnected graph with two components, *i.e.*.

$$L = L^- \cup L^+ \tag{6}$$

where L^- (L^+) is the component contructed solely of vertices of odd-parity (even-parity) and is defined by matrices $\boldsymbol{BB'}$ ($\boldsymbol{B'B}$). Obivously, their characteristic polynomials satisfy the following relation

$$P_L(y) = P_{L^-}(y)\, P_{L^+}(y) \tag{7}$$

with

$$y^{m-n}\, P_{L^-}(y) = P_{L^+}(y) \tag{8}$$

and y is the argument. Eq. (7), which looks like Eq. (1), reveals that the spectrum of L is the union of the spectra of L^- and L^+, whereas Eq. (8) indicates the isospectrality between L^- and L^+ up to $m - n$ zeros belonging to L^+.

It is known that endospectral points share absolutely equal coefficients for the nondegenerate eigenvectors,[28] *i.e.* if G is endospectral with k and k' being endospectral points, then

$$\left[c_k(G, x)\right]^2 = \left[c_{k'}(G, x)\right]^2 \tag{9}$$

As we know, eigenvectors are solved from the homogeneous linear equations formulated in the matrix form below.

$$(x\boldsymbol{I} - \boldsymbol{A})\, C = 0 \tag{10}$$

where $\boldsymbol{I}$ denotes the identity matrix, $C = C(G,x)$ is the column set of c's referring to eigenvalue x, as shown in Eq. (4); therefore, one can derive various formulae for c's with x as a variable. One of the formulae is listed below[35,42]

$$\left[c_\sigma(G, x)\right]^2 = P_{G-\sigma}(x) \tag{11}$$

where the right-hand side denotes the characteristic polynomial of graph $G - \sigma$ produced by erasing the σ-vertex from graph G. Eq. (11) makes Eq. (9) transform to

$$P_{G-k}(x) = P_{G-k'}(x) \tag{12}$$

giving a criterion for determining endospectral points, *i.e.* by inspecting whether $G - k$ and $G - k'$ are explicitly identical. But we may fail in other cases where $G - k$ and $G - k'$ look different.

It has been pointed out that the endospectral pair of G can be detected from its contracted graph C' as equivalent points if new symmetry elements occur in C',[34,35] so we concentrate in Eqs. (7) and (8). As we know, the characteristic polynomial of bipartite graph G is defined as follows

$$P_G(x) = \mathrm{Det}\,(x\boldsymbol{I} - \boldsymbol{A}(G)) = \mathrm{Det}\,(x\boldsymbol{I} + \boldsymbol{A}(G)) \tag{13}$$

regardless of the sign preceding the adjacency matrix in the determinant. For graph L, derived from G by the wrapping procedure, one has $\boldsymbol{A}(L) = (\boldsymbol{A}(G))^2$ and, if $y = x^2$, then

$$P_{L(G)}(y) = \mathrm{Det}\left(y\boldsymbol{I} - (\boldsymbol{A}(G))^2\right) = \left(P_G(x)\right)^2 \tag{14}$$

Based on Eq. (14), the following lemma is readily verified.

Lemma. If graphs Q and H are bipartite, $L(Q)$ and $L(H)$ are derived from Q and H by taking $(\boldsymbol{A}(Q))^2$ and $(\boldsymbol{A}(H))^2$ as adjacency matrices, respectively, then $L(Q)$, $L(H)$ are isospectral as long as Q and H are isospectral or *vice versa*, namely

$$P_Q(x) = P_H(x) \Leftrightarrow P_{L(Q)}(y) = P_{L(H)}(y) \tag{15}$$

Since G is bipartite, $G - k$ and $G - k'$ will be bipartite, too. On putting $Q = G - k$, $H = G - k'$ and combining Eq. (12) and Eq. (15), one arrives at the following theorem about endospectrality.

Theorem. If k and k' represent endospectral points of a bipartite graph G, then they are also endospectral points of $L(G)$, namely

$$P_{L(G)-k}(y) = P_{L(G)-k'}(y) \tag{16}$$

where the fact that $L(G-k)$ is identical to $L(G)-k$ has been used. The inverse statement is true too, that is, if Eq. (16) is satisfied, k and k' are endospectral points for G.

Endospectral points can be vertices of homo-parity or heteroparity. In the first case, we may suppose that both of them are odd, namely k and k' belong to $V^-(G)$, so $L^+(G-k) = L^+(G-k') = L^+(G)$. When combining Eqs. (16) and (7) so as to eliminate the common factor $L^+(G)$, the following equality results

$$P_{L^-(G)-k}(y) = P_{L^-(G)-k'}(y) \tag{17}$$

On the other hand, if k and k' are of odd- and even-parity, respectively, one may join Eqs. (16) and (7) and (8) together to derive another equality, as follows

$$y^{m-n}P_{L^-(G)-k}(y) = P_{L^+(G)-k'}(y) \tag{18}$$

These two equalities are fundamental to determining endospectral points that cannot be recognized simply by inspecting $G-k \not\cong G-k'$. They can be formulated as corollaries.

Corollary 1. For the bipartite graph G, its endospectral points can be simply determined if $L^-(G)-k = L^-(G)-k'$, where k, k' represent the endospectral pair of homo-parity and $L^-(G)$ is the component of $L(G)$ derived from G by the wrapping procedure.

Corollary 2. For the even bipartite graph, *i.e.* $m = n$, its endospectral points can be determined if $L^-(G)-k = L^+(G)-k'$, where k, k' denote the endospectral pair of hetero-parity with $k \in V^-(G)$ and $k' \in V^+(G)$, $L^+(G)$ is another component of $L(G)$ defined by $\boldsymbol{B'B}$ (see Eq. (5)).

Corollary 3. If $L^-(G)$ (or $L^+(G)$ is a symmetric graph, k and k' are equivalent vertices so that $L^-(G)-k = L^-(G)-k'$, k and k' are sure to be endospectral points for graph G.

Based on the principles presented above as a theorem and corollaries, we can now deal with the endospectrality for hexagonal graphs and other bipartite graphs in terms of how to recognize them and how to construct new species. In the following, we discuss endospectral points of homo-parity in detail and briefly account for hetero-parity species. Numerous novel endospectral graphs are tabulated.

ENDOSPECTRAL POINTS OF HOMO-PARITY

As early as in 1975, Herndon and Ellzey listed a dozen hexagonal graphs involving endospectral points.[28] More recently, Randić and coworkers[26] reported two additional examples: 1-methene-2-vinylphenanthrene and 6-methene benzo[cd]pyrene, displayed in Figure 2 under numbers 6, and 7, respectively. The graphs numbered 1 to 5 in Figure 2 are taken from Ref. 28. $L^-(G)$ and $L^+(G)$ for these graphs are displayed in the middle column of Figure 2, where open and solid circles signify the mono- and tri-valent vertices from the remaining di-valent vertices in graph G. In Figure 2, new symmetry elements occur in $L^-(G)$, so that $L^-(G)$ has higher symmetry than its parent graph G. Conventionally, these unmoved vertices under the new symmetry operations are called unrestricted points,[28] while the equivalent vertices under the new symmetry operations are endospectral points of G.

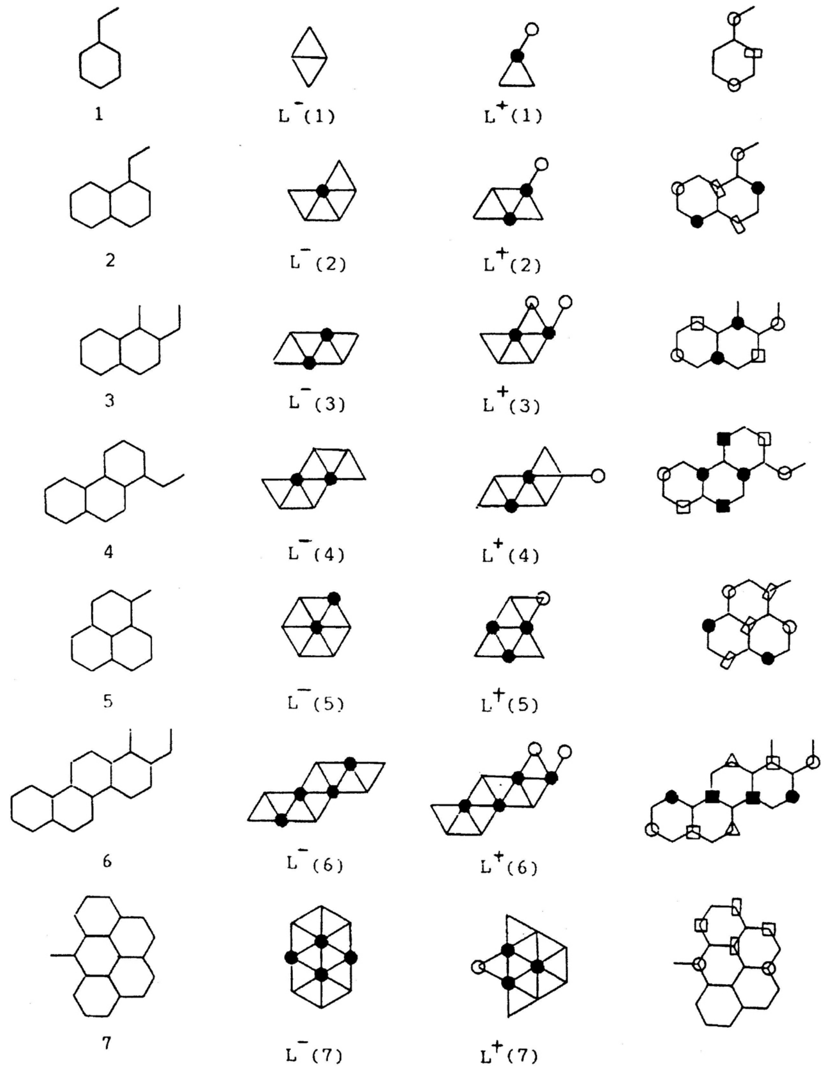


Figure 2. L^- and L^+ of seven endospectral graphs[26,28]

In Figure 2, $L^-(G)$ for 1, 2, 5 and 7 belong to point group C_{2v} or D_{2h} having two or more reflection planes, the numbers of endospectral pairs are equal to 1, 2, 3, and less than $n/2$ due to the existence of unrestricted points, whereas $L^-(G)$ for 3, 4, and 6 belonging to C_{2h} have exactly $n/2$ pairs of endospectral points because there is no unrestricted point. These results are shown schematically in the last column of Figure 2, where small rectangles represent unrestricted points and endospectral pairs are denoted by squares, triangles and circles in the open or solid style.

CONSTRUCTION OF ENDOSPECTRAL HEXAGONAL GRAPHS

From the discussions in the last section, we arrive at an important conclusion: the new symmetry elements occurring in $L^-(G)$ (or $L^+(G)$) are the source of endospectrality of the bipartite graph G. Some more examples are given in Figure 3. The benzyl graph can be transformed into L with component L^-, a triangle exhibits the same symmetry as its parent; L^- of the styrene graph possesses higher symmetry than its parent; the component L^- for naphthalene, which is a triply fused triangular graph (see Figure 3c) and belongs to C_{2v}, is less symmetric than naphthalene, whereas 1-vinylnaphthalene has lower symmetry than its derived component L^-. In consequence, styrene and 1-vinylnaphthalene are endospectral whereas benzyl and naphthalene are not, *i.e.* without endospectral points. This analysis sheds a valuable insight into the problem of how to construct endospectral bipartite graphs with pending bonds.

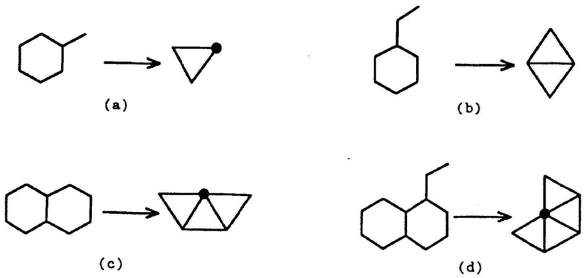


Figure 3. Influence of pending chains on L^-

If we consider anthracene in succession and draw its L^- (Figure 4), their symmetry are D_{2h} and C_{2v}, respectively, in analogy to naphthalene. On introducing three pending chains, new species 8, *i.e.* 1,9-dimethene-2-vinylanthracene, is formed. The derived component $L^-(8)$ of C_{2h} symmetry indicates that 8 bears four pairs of endospectral points. This procedure can be continued by introducing pending chains onto tetracene and pentacene to derive graphs 9 and 10 involving five and six pairs of endospectral points, respectively (see Figure 4). In this way, a general graph 11 representing the endospectral member derived from t-polyacene by joining up one ethene and $t-1$ methenes as pending chains is deduced. The $t+1$ pairs of endospectral points can be specified by the number set $(s, 2t+1-s)$ with $1 \leq s \leq t$ defined by the coordinate along the line below 11 in Figure 4.

Furthermore, one may find two different endospectral series from zigzag polyacenes. The first series is characterized by the occurrence of a pending ethene and can be regarded as homologues of styrene in which the chain of hexagon propagates zigzagly where the small members with $h \leq 3$ (h means the number of hexagons) have appeared in Figure 2 as graphs 1, 2 and 4, medium ones with $h = 4, 5$ are given in Figure 5, as 12 and 13. Among them, odd-membered species ($h = 1, 3, 5,...$) contain $h + 1$ (or $n/2$) pairs of endospectral points and two unrestricted points in relation to the symmetry of L^-. The second series is an extension of graphs 3 ($h = 2$) and 6 ($h = 4$) in Figure 2, so one can easily draw the other members of the series, such as 14 ($h = 3$)

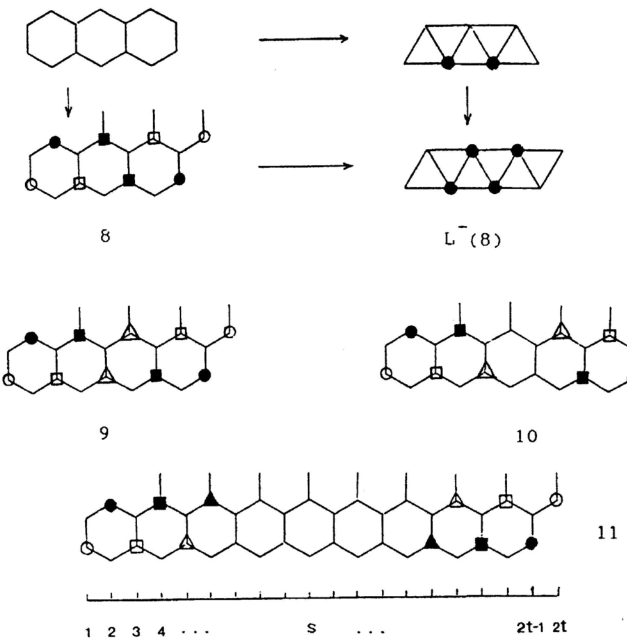


Figure 4. The endospectral series derived from polyacenes

and 15 (h = 5) given in Figure 5. In contrast to the first series, the even-membered graphs 3 and 6 involve h + 1 pairs or endospectral points due to the C_{2h} symmetry of $L^{-}(3)$ and $L^{-}(6)$, but the odd-membered species 14 and 15 have two unrestricted points besides h pairs of endospectral points because the corresponding Ls are of C_{2v} symmetry.

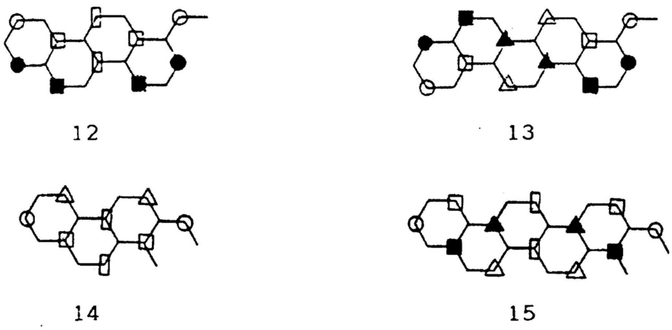
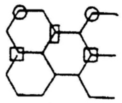


Figure 5. Lower members of the endospectral homologous series derived from zigzag polyacenes.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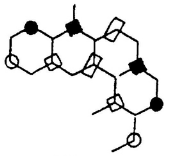
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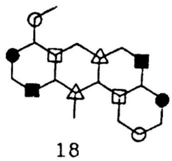
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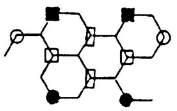
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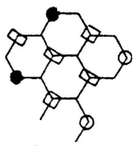
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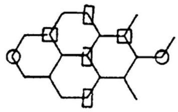
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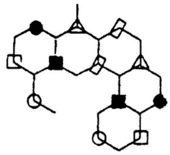
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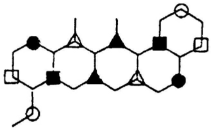
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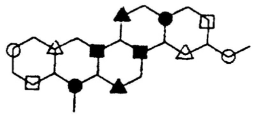
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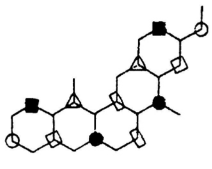
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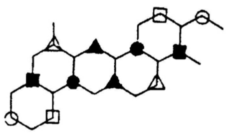
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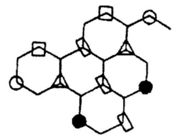
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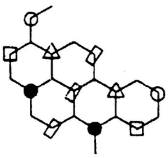
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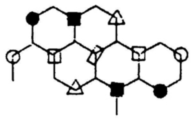
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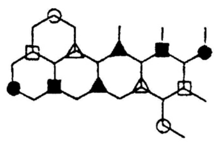
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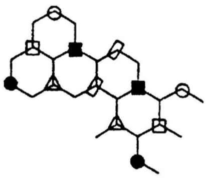
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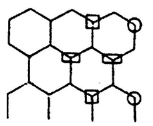
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Figure 6. Some endospectral graphs derived from benzenoids with $h \leq 5$.

By the same procedure, we can examine various systems of cata- and pericondensed benzenoids in order to find more endospectral graphs still unknown. Results of $h \leq 5$ are displayed in Figure 6.

PERICONDENSED HEXAGONAL GRAPHS

Two pericondensed graphs 5 and 7 have been displayed in Figure 2, where the resemblance between diagrams $L^{-}(5)$ and $L^{-}(7)$ is quite clear. Actually, graph 7 can be regarded as the entity generated from 5. Another perifused member is graph 33 with L^{-} (33) quite similar to $L^{-}(7)$; their distribution of endospectral pairs and un-

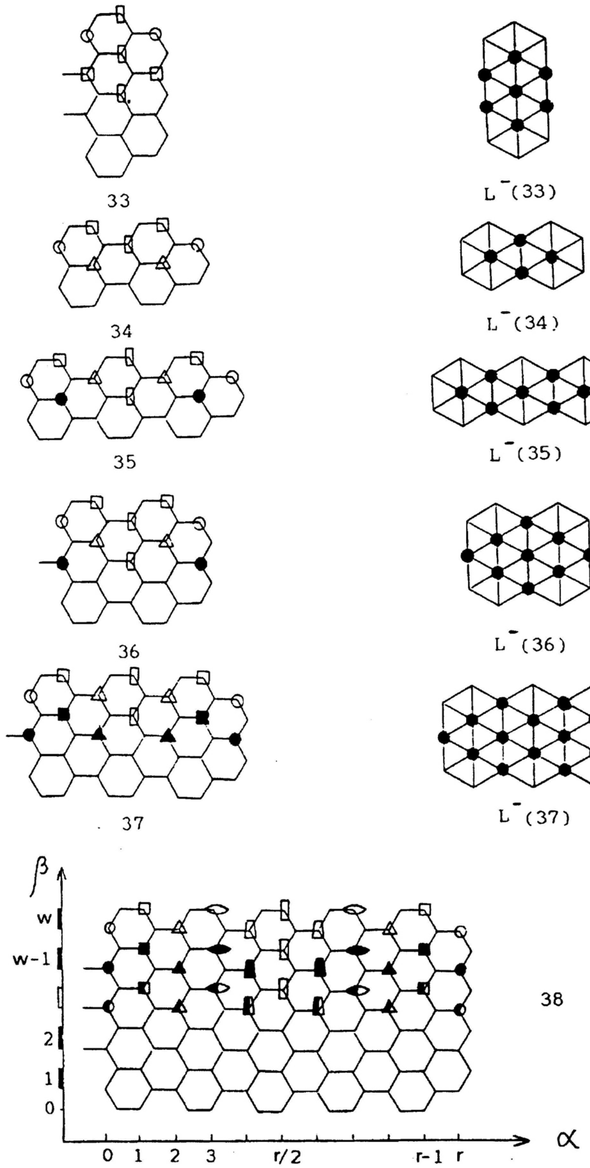

Figure 7. Endospectral graphs of hexagonal lattice derived from graphs 5 and 7.

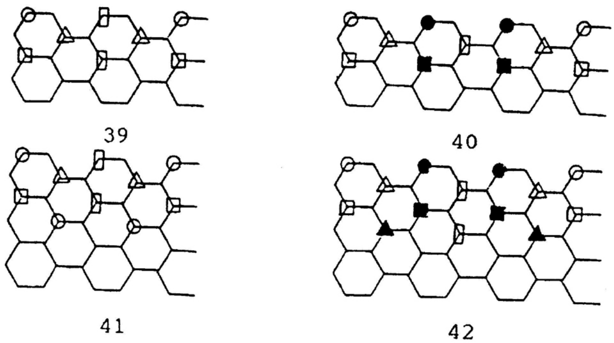

Figure 8. Homologues of endospectral graphs derived from graphs 16 and 32.

restricted points are shown in Figure 2 and Figure 7. Surely, huger members of this homologous series can be readily deduced. Graphs 34, 35 are species produced by another propagation pattern from graph 5. They are endospectral due to the D_{2h} symmetry of $L^{-}(34)$ and $L^{-}(35)$. A similar process starting from graph 7 leads to graphs 36, 37 and even larger analogues which are endospectral in consistence with the common symmetry of their L^{-}s (see Figure 7). In general, both ways of propagation can take place simultaneously, resulting in a planar lattice, graph 38 of length r and width w with $w - 2$ pending methenes along the width. A coordinate system is introduced aside graph 38 where α and β characterize the vertex set $V^{-}(38)$; then, (α,β) specifies a definite vertex of ood-parity with $0 \le \alpha \le r$ and $0 \le \beta \le w$. Graph 38 is endospectral as long as r is an even number, and it can be represented by the pair $[r, w]$, so graph 7 and graphs 34 to 37 can be denoted by [2, 3], [4, 2], [6, 2], [4, 3] and [6, 3], respectively. In graph 38, each pair of endospectral points is in the position of (α, β) and $(r - \alpha, \beta)$, and the w unrestricted points are located on the line with $\alpha = r/2$.

It is worth noting that there are endospectral species (such as 34 and 35) without pending chains, revealing that pending chains occur frequently but not necessarily in the endospectral cyclic bipartite graphs.

In the same way, one may discern the analogy between graphs 16 and 32, and then derive another homologous series of endospectral graphs displayed in Figure 8.

The one-dimensional hexagonal graph 11 can propagate vertically in zigzag manner, resulting in another endospectral lattice (with one pending ethene and $w - 1$ pending methene on the top border) where the horizontal and vertical lengths of the lattice are w and r, respectively. Thus, one can use the number pair $[r, w]$ to specify each member of this homologous series. Due to the C_{2h} or D_{2h} symmetry of $L^{-}(r, w)$, members with even r (such as graphs 43 and 47) contain unrestricted points along the midst horizontal, but others with odd r (graphs 48 to 50) involve only endospectral points. They are displayed in Figure 9.

We have discussed three families of hexagonal lattice that are endospectral with the zigzag boundary along the direction of length. Is it a necessary condition? The answer is 'no'. Let us consider the fourth example, a parallelogram-like lattice graph of lengths r and w with a similar distribution of pending chains along two sides as

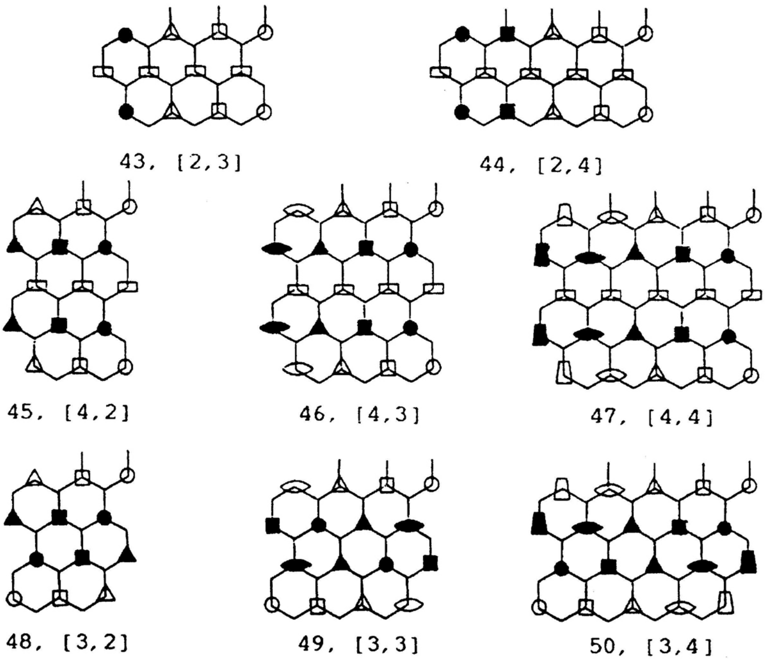

Figure 9. The endospectral series of lattice type derived from graph 11.

in graph 10. In this homologous series, $L^{-}(r,w)$ has symmetry C_{2h} if $r \neq w$ and D_{2h} if $r = w$, all of them are endospectral with unrestricted points occurring in members with $r = w$. In Figure 10, three species with $r = 3$ and $w = 2, 3, 4$ are displayed.

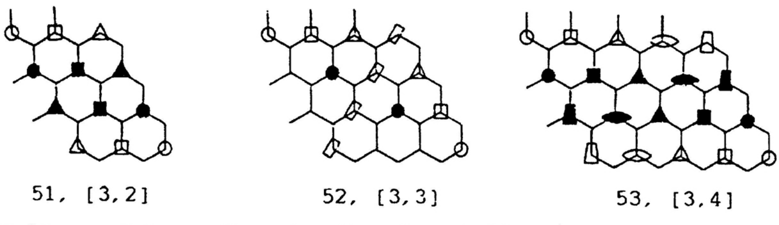

Figure 10. The parallelogram-like polycyclic endospectral homologues.

ENDOSPECTRAL POINTS OF HETERO-PARITY

There are also endospectral points of hetero-parity for bipartite graphs, most of which are trees,[38] and so far only one cyclic species, 54, is available.[28,33] In Figure 11, we draw $L^{-}(54)$ and $L^{+}(54)$ where squares signify the endospectral points k and k'. It can easily be seen that $L^{-}(54) - k = L^{-}(54) - k'$, so that Eq. (17) is satisfied. Of course, more graphs of such type can be found by our methods. Thus, graphs 55, 1,2-divinyl-

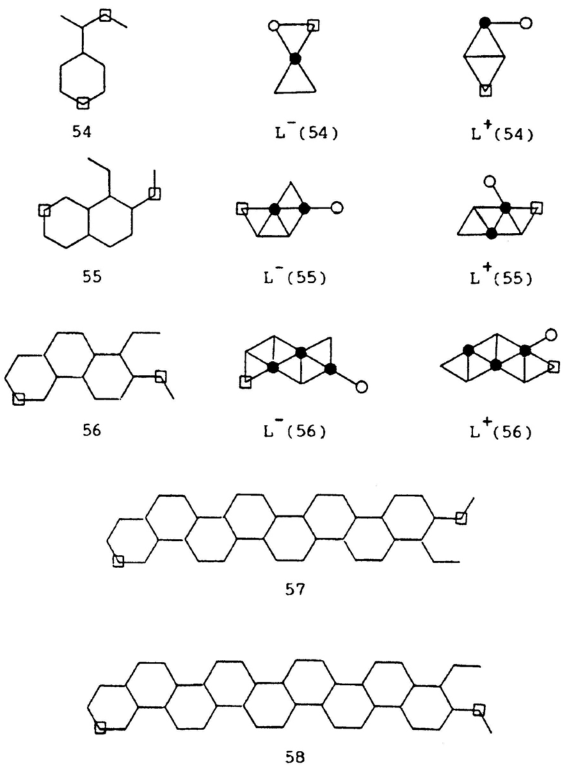

Figure 11. Derivatives of zigzag polyacene with a pair of endospectral points of hetero-parity.

naphthalene and graph 56 are endospectral under the same constraints, *i.e.* $L^{-}(55) - k = L^{+}(55) - k'$ and $L^{-}(56) - k = L^{+}(56) - k'$. By deduction, a homologous series, which is derived from zigzag polyacene joining up with pending chains and involving endospectral points of hetero-parity, can be constructed. Typical members consisting of even and odd hexagons, 57 and 58, are given in Figure 11.

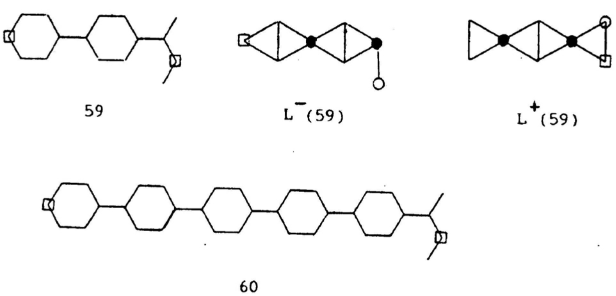

Figure 12. Derivatives of poly-*p*-phenyls with a pair of endospectral points of hetero-parity.

Another homologous series can be constructed from graph 54, and graph 59 is the second member satisfying $L^{-}(59) - k = L^{+}(59) - k'$ with k and k' represented by squares in the diagram of Figure 12, so graph 59 involves a pair of endospectral points of hetero-parity. Graph 60 can be taken as a typical member of this homologous series.

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SAŽETAK

O endospektralnim bipartitnim grafovima

Yuansheng Jiang i Chenzhi Liang

Predložen je novi pristup detektiranju i konstrukciji endospektralnih bipartitnih grafova. Navedeno je više od 50 novih vrsta i obitelji endospektralnih parova sastavljenih od šesterokutnih rešetaka. Također su opisana i pravila na koji su način ti endospektralni grafovi konstruirani.