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THE CONSTRUCTION OF ISOSPECTRAL GRAPHS

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Abstract. Five general procedures for constructing pairs of isospectral graphs are delineated. The concepts of isospectral points and unrestricted points in a graph are recapitulated, and methods for constructing graphs with these features are described. The concept of an infinite pair of isospectral graphs is illustrated. Nonregular isospectral pairs of graphs whose complementary graphs are also isospectral are discussed. The concepts and methods are utilized in the construction of numerous pairs of isospectral graphs, including the smallest known isospectral pair with six vertices, the smallest pair without pendant edges, and 18 of the 33 known isospectral pairs with seven vertices.

I. Introduction

Isospectral graphs, sometimes called cospectral graphs, are graphs which are not isomorphic, but whose adjacency matrices have the same eigenvalue spectra.[1] The concept of isospectrality is of particular interest in chemical applications of graph theory where graphs, both labeled and unlabeled, are universally used to represent molecular structures.[2-5] In some cases the eigenvalues of the matrix $H = \alpha I + \beta A$, where I is the identity matrix, A is the adjacency matrix of a molecular graph, and α and β are appropriate parameters, correspond to observable quantities. For example, in Hueckel molecular orbital theory, these eigenvalues are the energies of the pi molecular orbitals of unsaturated hydrocarbons.[6] It has also been shown that these eigenvalues can yield good approximations to the vibrational frequencies of certain linear and ring compounds when H is identified with the GF matrix.[7] Because of these applications, methods for finding or constructing isospectral graphs have some practical relevance, along with intrinsic interest as a graph theory problem.

The existence of isospectral graphs also has relevance to problems in coding and storage of chemical structures. At one time, it was postulated that the eigenvalue spectrum of the adjacency matrix of a graph was a unique property of that graph.[8,9] However, the existence of isospectral graphs negated this conjecture.[9] Later it was proposed that if a molecular graph were labeled with appropriate symbols and the secular polynomial obtained as a determinant, this polynomial would be unique.[10,12] This also turned out to be incorrect.[9,13,14] In fact, one completely general algorithm was published that allowed one to construct pairs of isospectral labeled graphs no matter the degree of labelling.[14] Method 8.1 (see later in this paper) presents a variation of that algorithm applied only to cases of unlabeled graphs. Although the general methods for constructing pairs of isospectral graphs can, for the most part, be easily adapted to labeled molecular graphs, the exposition in the present paper will be restricted to unlabeled cases. The necessary elaborations for extension to labeled or weighted graphs will be evident in context.

The problem of finding isospectral weighted graphs is trivial in the sense that any two graphs corresponding to equivalent adjacency matrices are necessarily isospectral. Thus, if W_1 is the adjacency matrix of a weighted graph G_1 and if S is a nonsingular conformable matrix, then the matrix $W_2 = S^{-1}W_1S$ will necessarily have the same eigenvalue spectrum as W_1. If the weighted graph G_2 corresponding to W_2 is not isomorphic to G_1, then G_1 and G_2 are isospectral. The only interesting problem is establishing the nonisomorphism of G_1 and G_2.

For nonweighted graphs, the problem of obtaining isospectral sets is not as easily dismissed. Of course it is true that many pairs and larger sets of isospectral graphs were discovered either by chance or by exhaustive examination of graphs of a particular size.[7,15,16] However, an interest in construction methods is manifested by a substantial number of published papers in which procedures to derive isospectral graphs have been outlined.[15-29] The purpose of this present paper is to list and give examples of several construction methods that we have found useful. In some cases, a resemblance to some of the other published procedures will be noted. In part, this may be due to the fact that the general combinatorial graph properties that allow the existence of isospectral graphs seem to be quite limited. Be that as it may, our final conclusion is that all (or nearly all) examples of isospectral graphs may be constructable.

II. Secular Polynomials

Isospectral graphs necessarily have indentical secular polynomials. Therefore procedures that allow one to obtain the secular polynomial from structural properties of the graph[11,30-36] are useful to help demonstrate that two nonisomorphic graphs are isospectral. Some other useful properties related to the secular polynomial are also reviewed in this section.

The secular polynomial of a graph G with adjacency matrix **A** is given by the determinant

$$P(G) = \det(A - \lambda I)$$

$$= a_n\lambda^n + a_{n-1}\lambda^{n-1} + \ldots + a0 \qquad (2.1)$$

where I is the identity matrix. The eigenvalues are the roots of the secular equation

$$P(G) = 0 \qquad (2.2)$$

Since the eigenvalues of **A** are the roots of the secular equation, (2.2), the secular polynomial can be expressed as

$$P(G) = (\lambda - E_1)(\lambda - E_2) \ldots (\lambda - E_n) \qquad (2.3)$$

and the adjacency matrix itself satisfies the secular equation

$$a_nA^n + a_{n-1}A^{n-1} + \ldots + a_0I = 0 \qquad (2.4)$$

Therefore, the coefficients of the secular polynomial are determined by the traces of the first n powers of **A**. Two simple graphs, G_1 and G_2, are consequently isospectral if and only if

$$\text{trace}(A_1)^k = \text{trace}(A_2)^k,\ k = 1, 2, \ldots, n \qquad (2.5)$$

These traces are called the spectral moments of the graphs. Relationships between random walks, spectral moments, and isospectral graphs have been delineated by Randić.[37]

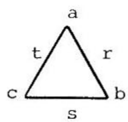
Decomposition techniques of Heilbronner,[38] originally developed for Hueckel molecular orbital theory have been usefully applied to the spectral study of graphs. Suppose a graph G is composed of two subgraphs G_1 and G_2 joined only by an edge between vertex p_1 in G_1 and vertex p_2 in G_2.

Heilbronner showed that the corresponding secular polynomials obey

$$P(G) = P(G_1)\, P(G_2) - P(G_1-p_1)P(G_2-p_2) \tag{2.6}$$

where G_1-p_1 represents graph G_1 with vertex p_1 and all its connecting edges removed. This algebraic device can be used to demonstrate isospectrality of two graphs by reducing their secular polynomials to polynomials of known isospectral or identical subgraphs.

For a labeled graph, the elements of the adjacency matrix are symbols corresponding to the labels of the vertices and edges as shown in fig. 2.1.



$$\begin{bmatrix} a & r & t \\ r & b & s \\ t & s & c \end{bmatrix}$$

Fig. 2.1. Labeled graph and adjacency matrix.

The secular polynomial of this graph is

$$P(\lambda) = xyz + 2rst - xs^2 - yt^2 - zr^2 \tag{2.7}$$

where $x = a - \lambda$, $y = b - \lambda$ and $z = c - \lambda$. It may not be possible to factor this polynomial completely.

III. Eigenvectors

The i^{th} eigenvector of **A**, v^i, corresponding to the i^{th} eigenvalue, E_i, satisfies the equation

$$Av^i = E_i v^i \tag{3.1}$$

The adjacency matrix, **A**, is symmetric. Consequently, its eigenvalues are real and its eigenvectors corresponding to different eigenvalues are orthogonal. Moreover, the eigenvalue relation can be written in terms of the nonsingular matrix V, whose columns are the eigenvectors of A, and the diagonal eigenvalue matrix E according to

$$AV = VE \tag{3.2}$$

The sum of the eigenvalues equals the trace of A, and the product of the eigenvalues equals the determinant of A.

Relations (3.2) can be rewritten as

$$A = VEV^{-1} \tag{3.3}$$

suggesting that a simple reordering of the eigenvalues along the diagonal of E would produce a new adjacency matrix isospectral to the first. Unfortunately, there is no guarantee that the graph of the new adjacency matrix would be simple.

IV. Isospectral Points

We have defined isospectral points of a graph to be two or more points such that deletion of one of the isospectral points yields a graph which is isospectral to the graph resulting from deletion of one of the other isospectral points. The resulting graphs are not necessarily connected. A classic example is provided by the indicated vertices of Schwenk's graph[15] shown in fig. 4.1.

$$(x^3 - 2x(x^5 - 4x^3 + 2x)$$

$$(x)(x^7 - 6x^5 + 10x^3 - 4x)$$

Fig. 4.1. Schwenk's graph with two isospectral points.

where the secular polynomials for the resulting graphs are also depicted. It follows from Heilbronner's theorem that attachment of any moeity to one of the isospectral points yields a graph which is isospectral to the graph resulting from attachment to one of the other isospectral points as exhibited in fig. 4.2.

Figure 4.2. Nonisomorphic isospectral graphs.

We have also proved a theorem concerning coefficients of isospectral points in adjacency matrix eigenvectors.[17]

Theorem: Let v_k^{ir} be the coefficient of the k^{th} point in the r^{th} degenerate eigenvector of A corresponding to eigenvalue E_i with degeneracy R. Then points k and l of G are either isospectral or equivalent if and only if

$$\sum_r^R (v_k^{ir})^2 = \sum_r^R (v_l^{ir})^2, \; i = 1, 2, \ldots, n \tag{4.1}$$

For the nondegenerate case, R = 1, relation (4.1) reduces to

$$(v_k^i)^2 = (v_l^i)^2, \; i = 1, 2, \ldots, n \tag{4.2}$$

which can be restated as

$$|v_k^i| = |v_l^i|, \; i = 1, 2, \ldots, n \tag{4.3}$$

Although it is important to identify and discard equivalent points-- points related by symmetry transformations-- this theorem can be a powerful tool for identifying isospectral points since it allows such points to be identified from examination of tables of HMO eigenvector coefficients. Other coefficient regularities observed for isospectral graphs have been reviewed, and have been used in several discussions of isospectral graph structure relationships.[18,19,25,26]

V. Unrestricted Substitution Points

An unrestricted substitution point is a graph vertex at which a substitution of any kind yields a graph in which the vertices which were isospectral in the original graph are also isospectral in the new graph.[16,17,39] Examples are vertices number 4 and number 8 in the styrene graph in fig. 5.1.

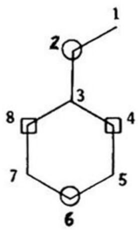


Fig. 5.1. Isospectral [○] and unrestricted [□] substitution points.

Using isospectral and unrestricted substitution points it is possible to generate any number of isospectral graphs beginning with only a few small graphs. Some examples of such processes will be given in sections VIII to XII.

VI. Composition Methods for Pairs of Isospectral Graphs

Method 6.1. Take two sets of $n + m$ ($n + m > 2$) copies of any graph A. Join points indexed j, k, l, etc., in n copies of A to points q, r, s, etc., in m copies of A to form a graph. Then join points q, r, s, etc., in n copies of A to points j, k, l, etc., in m copies of A to form a second graph. The two composed graphs are nonisomorphic and isospectral.

The graph A may not be L_1.[40] The sets of points j, k, l, etc., must be distinct from q, r, s, etc., and n must differ from m. However, some of the points in the two sets may be identical. In the examples to be given the starting components of the graph will be are shown by heavy lines, and the joining edges are the lighter lines.

The six and eight point pairs of graphs in fig. 6.1 are the smallest

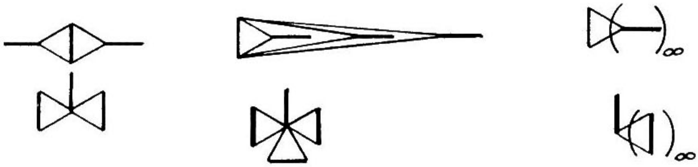


Fig. 6.1. Isospectral graphs constructed from L_2.

obtainable isospectral pairs using method 6.1 and L_2 as the prototype graph. The 6-vertex pair is the smallest pair of isospectral connected graphs, first reported by Baker.[7] One can see that the series starting with the pairs shown in Fig. 6.1 is an infinite family, so that pairs of isospectral graphs with any even number of vertices larger than 6 are available using L_2 and 6.1. The number of pairs of isospectral graphs that can be composed from n + m copies of L_2 (two sets) is $(n + m - 1)/2$ if n + m is odd, and $(n + m - 2)/2$ if n + m is even. One also realizes that there must exist pairs of infinitely large nonisomorphic isospectral graphs, the pair based on L_2 to be represented as in fig. 6.1. To our knowledge, no examples of infinite isospectral graphs have been previously studied.

There are over 20 9-vertex graphs that can be composed using method 6.1 and either L_3 or C_3 as the starting graph. The single pair of tree graphs that can be constructed in this way and a few of the other pairs are shown in fig. 6.2.

<u>Method 6.2.</u> Take two sets of n (n odd) copies of any graph A. Number the graphs 1 through n. Form a larger graph by joining points indexed j, k, l,

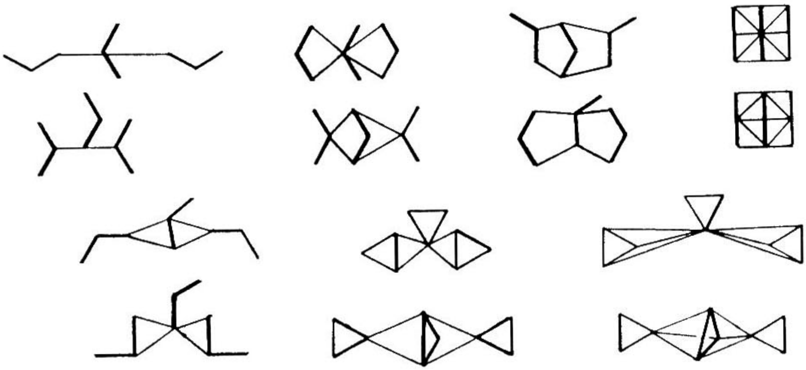


Fig. 6.2. Pairs of isospectral 9-point graphs based on L_3 and C_3.

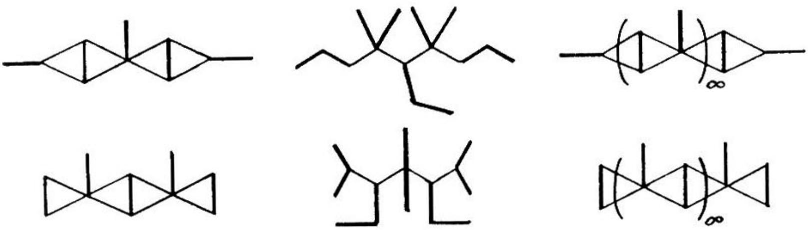


Fig. 6.3. Isospectral graphs constructed using method 6.2.

etc., in even numbered graphs to points indexed q, r, s, etc., in odd numbered graphs, no graphs to be joined to other than their nearest neighbors. Carry out the complementary procedure to form a second graph isospectral to the first. Examples are given in fig. 6.3.

VII. Expansion of Bipartite Graphs

Method 7.1. Star the vertices of a bipartite graph so that no two starred vertices are connected by an edge. If the number of starred positions equals the number of unstarred positions and they are not equivalent by symmetry, add any graph, first to each starred position, then to each unstarred position, to obtain two nonisomorphic isospectral graphs.

Equivalence as used above is to be taken in the structural sense. For example, in any linear even bipartite graph the unstarred and starred positions are equivalent and isospectral graphs cannot be constructed using 7.1.

The smallest bipartite graphs with the required nonequivalent starred and unstarred positions have 6 points and are given in fig. 7.1, along with

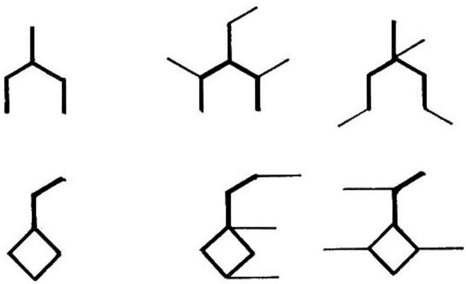


Fig. 7.1. Isospectral graphs from expansion of bipartite graphs.

the expanded 9-vertex isospectral pairs obtainable by adding L_1 to each separate set of vertices. The isospectral tree graphs in fig. 7.1 were also constructed using method 6.1, as depicted in fig. 6.2.

VIII. Construction of Graphs with Isospectral and Unrestricted Points

It is important to understand that the complementary graph of any graph with isospectral points possesses the same isospectral points. The potential pool of isospectral pairs of graphs obtainable by use of isospectral points is therefore doubled. However, since the complementary graphs of two isospectral graphs are not generally themselves isospectral, the complementary graph with isospectral points must first be obtained, with subsequent formation of the isospectral pair by coalescence with other graphs. See section XI for a discussion of complementary graphs of isospectral pairs formed by deletion of isospectral points. All of the concepts are best clarified with examples, and several will be shown below. Then we will give two general methods for constructing graphs with isospectral and unrestricted points, and list additional properties that are useful in constructing isospectral graphs.

The 8-point graphs listed in fig. 8.1 are the smallest graphs with isospectral points, indicated by circles. The styrene graph in fig. 8.1 also has two unrestricted substitution points, indicated by squares. In

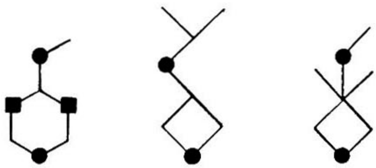


Fig. 8.1. Graphs with isospectral points.

that graph, deletion of an unrestricted substitution point converts the isospectral points to equivalent points. Isospectral pairs containing 9 or 10 points that can be generated from the graphs in fig. 8.1 are pictured in fig. 8.2. Infinite numbers of isospectral pairs of any size larger than 8 vertices are available using the starting graphs in fig. 8.1.

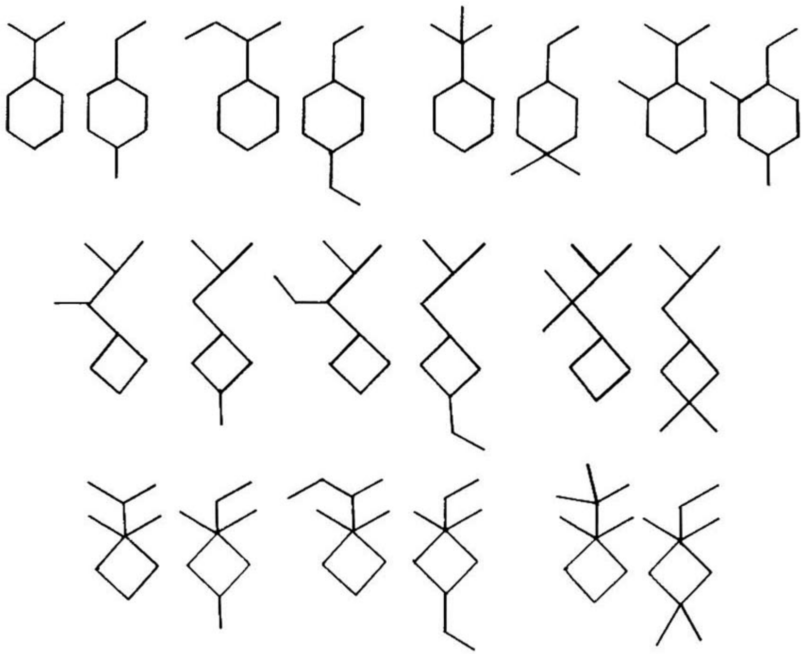


Fig. 8.2. Isospectral graphs from isospectral points.

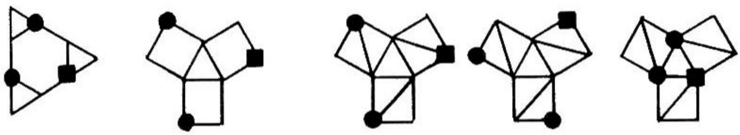


Fig. 8.3. Isospectral and unrestricted substitution points.

Method 8.1. Use of n-fold symmetry. Take a graph containing points a, b, c, etc., that are related by an n-fold axis of symmetry (n > 2), and which are not related by two-fold axes of symmetry. Delete point b or join any graph to point b to generate isospectral points a and c.

The points a, b, c, etc., are required by symmetry to have identical absolute values of eigenvectors. The pairwise reciprocal relationships a-b, b-c, etc., are also identical from symmetry considerations. Substitution at b destroys the n-fold symmetry of the graph, but has an identical effect on the eigenvectors of a and c. The points a and c are therefore isospectral and can be used to generate pairs of isospectral graphs. Proofs of the preceding assertions can be obtained using various HMO theorems and definitions given by Coulson and Longuet-Higgens.[41]

The smallest graphs that correspond to the requirements of method 8.1 have 3-fold symmetry and 9 points. Three basic structures are outlined in fig. 8.3, where circles and squares indicate potential isospectral and unrestricted substitution points respectively. The complementary graphs are very complicated and are not shown. The third example shows that a single graph may have several sets of isospectral and unrestricted points. Pairs of 9-point isospectral graphs are available by initial deletion of the unrestricted substitution points and joining of L_1 at one and then the other of the two isospectral points. An example of such 9-point pairs is given in fig. 8.4.

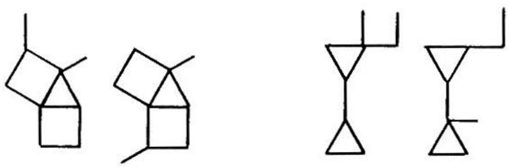


Fig. 8.4. Isospectral graphs constructed using method 8.1.

Method 8.2. A decomposition principle. We have found one additional way to generate graphs with isospectral points. In certain graphs, the generalized form of which is shown in fig. 8.5, there are two particular vertices

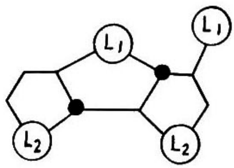


Fig. 8.5. Generalized graph with isospectral points.

related by a pseudo-symmetric element in that deletion of one vertex generates an identical graph to that formed from deletion of the other vertex. The two points are therefore isospectral points. Examples of graphs with isospectral points of this type are listed in fig. 8.6. Again,

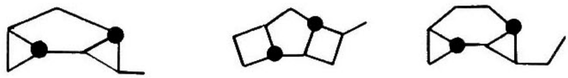


Fig. 8.6. Graphs with isospectral points.

the smallest graph of this type has eight points so that (considering the complementary graph) two 9-point isospectral pairs can be constructed.

IX. Properties of Isospectral and Unrestricted Points

Schwenk's graph, fig. 4.1, with two isospectral points, and the first graph in fig. 8.1, with isospectral and unrestricted substitution points, will be used to illustrate the properties of isospectral and unrestricted points. Several of the properties have to do with the maintenance of isospectral points after coalescence with other graphs or addition of lines (new edges) to the graph. In the context of this work, the importance of such alterations is that each change creates a new graph that can be used to generate pairs of isospectral graphs. Alteration rules are as follows.

9.1. Attachment of identical graphs simultaneously at isospectral points leaves the points isospectral.

9.2. Attachment of isospectral points to each other leaves the points isospectral.

9.3. Attachment of isospectral points to a single point, equivalent, or isospectral points in a second graph leaves the original points isospectral.

9.4. Attachment of unrestricted substitution points to each other maintains the isospectral points.

9.5. Attachment of unrestricted substitution points to isospectral points simultaneously maintains the isospectral points.

9.6. Attachment of unrestricted points through any graphical moiety to isospectral points simultaneously maintains the isospectral points.

Rules 9.1 to 9.4 are illustrated in fig. 9.1 below, and rules 9.5 and 9.6 are exemplified in fig. 9.2.

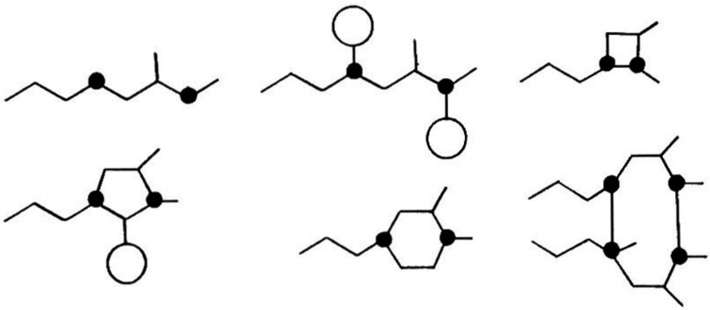


Fig. 9.1. Graphs with isospectral points derived from Schwenk's graph.

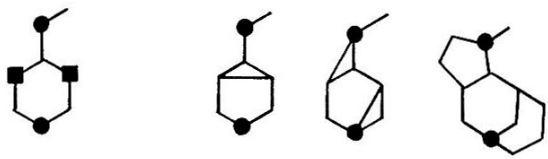


Fig. 9.2. Graphs with isospectral points.

9.7. For bipartite graphs only, the vertices adjacent to isospectral points may be attached to one another directly or through any second graph without affecting isospectrality of the isospectral points. For nonbipartite graphs, adjacent vertices may not be directly attached, but attachment through a single vertex in a second graph is allowed. Examples are given in fig. 9.3.

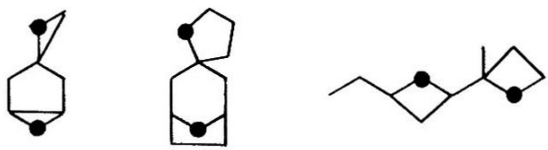


Fig. 9.3. Graphs with isospectral points.

X. Construction of Isospectral Graphs Using Isospectral Points

Isospectral points may be located by trial and error, by examination of eigenvectors, or may be created as described in VIII. The graphs with isospectral points may be altered as shown in section IX with retention of the isospectral points. More than one of the procedures in section IX can be applied simultaneously. Then, in addition to the fact that isospectral pairs of graphs can be constructed by sequential coalescence of any graph at isospectral points, the following two methods can also be used.

Method 10.1. Two different graphs attached to two isospectral points in a reciprocal relationship generate pairs of isospectral graphs, as shown in fig. 10.1.

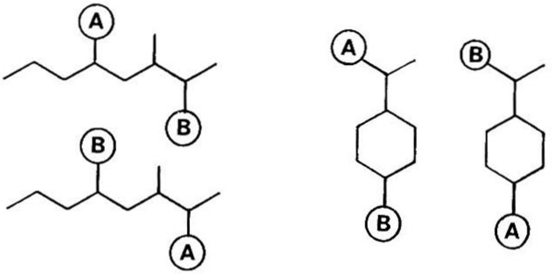


Fig. 10.1. Isospectral graphs from reciprocal disubstitution.

Method 10.2. The procedures outlined in 9.5 through 9.7, if applied to the two isospectral points separately in two copies of the original graph, generate pairs of isospectral graphs. Examples are shown in fig. 10.2. One can see that a very large number of pairs of isospectral 8-point graphs are thus available.

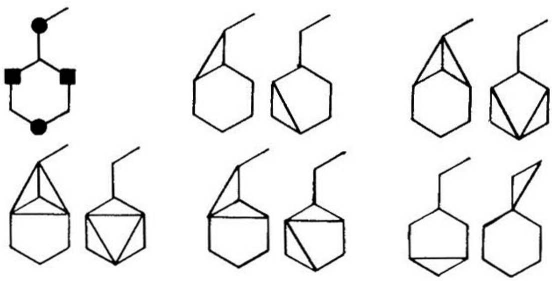


Fig. 10.2. Isospectral pairs of 8-point graphs.

XI. Isospectral Graphs From Deletion of Isospectral Points

Method 11.1 Deletion of isospectral points from a graph in turn, where the resulting graphs are not disconnected or identical, gives a pair of isospectral graphs.

Method 11.2 The complementary graphs of a pair of isospectral graphs that were constructed using 11.1 are themselves isospectral if they are connected graphs.

It can easily be demonstrated that if two nonisomorphic graphs have the same characteristic polynomial (are isospectral) and are regular, their complements also have the same polynomial. Method 11.2 indicates that there is an additional class of pairs of isospectral graphs that are not regular but whose complements are isospectral. Examples using methods 11.1 and 11.2 will be given in section XII.

XII. Isospectral Graphs With 7 Points

A number of the methods using isospectral and unrestricted substitution points can be illustrated by the construction of isospectral 7-point graphs. Such graphs have been exhaustively enumerated by Harary, et al.[8] There are no isospectral tree graphs with 7 points, and there are 33 connected isospectral pairs containing cycles. We think it interesting that 16 of these isospectral pairs are constructible from a single precursor, the 8-point bipartite styrone graph in fig. 8.1 with two isospectral points and two equivalent unrestricted substitution points. The syntheses of these 7-point isospectral pairs of graphs are outlined in figs. 12.1, 12.2, and 12.3. The generally used procedure was to employ rule 9.7 first, then 9.4 and 9.5. Subsequent deletion of the maintained isospectral points according to 11.1 then gives a pair of isospectral graphs. The six pairs shown in fig. 12.1 also have complementary graphs that are isospectral in pairs, giving altogether 12 pairs of isospectral graphs. The last pair in

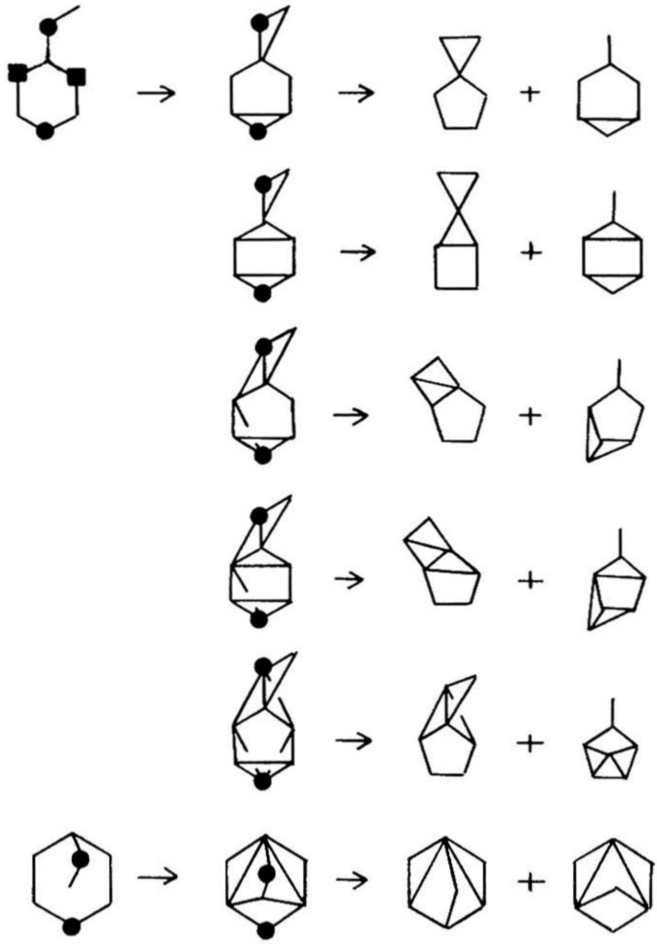


Fig. 12.1. Isospectral pairs of 7-point graphs.

fig. 12.1 is the previously reported smallest pair of isospectral graphs without pendant edges.[8]

The complete graph with seven points has 21 edges. If the procedure outlined above gives isospectral graphs with more than ten points, it is possible that a pair complementary to one of the already synthesized pairs might be obtained. The graphs in fig. 12.2 are obtained by further use of the outlined procedure, and do give isospectral graphs with more

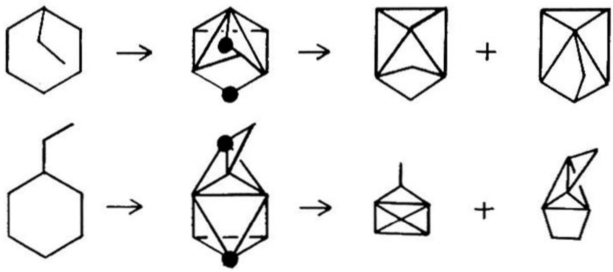


Fig. 12.2. Isospectral graphs complementary to graphs in Fig. 12.1.

than 10 edges that prove to be the complementary graphs to the fifth and sixth pairs respectively in fig. 12.1. Therefore, no additional pairs of isospectral graphs have been constructed.

Continuing the procedure, one obtains the pairs with 12 and 14 edges shown in fig. 12.3 These pairs cannot be the complementary graphs of any one of the pairs in fig. 12.1, because the right-hand graph in each case contains a vertex connected to every other vertex. Its complementary graph would be disconnected, which is not true for the graphs in fig. 12.1. However, the second and third isospectral pairs of fig. 12.3, are identical, so only three new isospectral pairs of graphs have been constructed.

Further isospectral pairs might be available using the prototype graph of fig. 8.1. If the isospectral points are each deleted in turn without

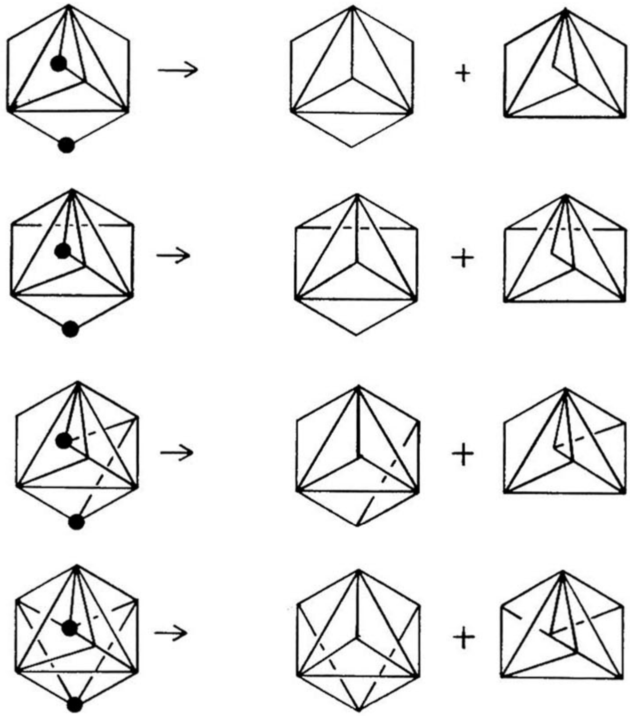


Fig. 12.3. Three pairs of isospectral seven-point graphs.

joining adjacent points, graphs with identical characteristic polynomials are created, but one of the graphs is disconnected. However, the complementary graphs are connected and could, therefore, constitute a new pair of isospectral graphs. The pair of graphs in fig. 12.4 was constructed by this type of procedure using the isospectral points without alteration in the original graph. Since these constructed isospectral graphs must have 15 edges, they are not isomorphic to any of the former graphs, and so one new isospectral pair is available in this way.

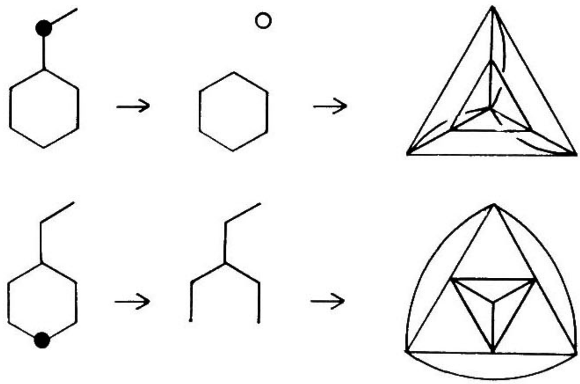


Fig. 12.4. A pair of 15-edge, seven-point isospectral graphs.

The eight-point graphs in fig. 8.1 with 4-membered rings allow the construction of two more pairs of 15-edge isospectral graphs. The procedure outlined is to delete the isospectral points in turn and form the complementary graphs as demonstrated in fig. 12.5. A check for nonisomorphism with the previously obtained seven-point graphs is, of course, not necessary, because of the method of construction.

Altogether, we have constructed 18 of the 33 isospectral pairs with seven points from precursor graphs with isospectral points. The several other procedures we outlined are not applicable to the seven point cases. For example, the composition principles given in VI are not applicable since seven is a prime number, and bipartite precursors to seven point graphs using the expansion method of VII are not possible. However, as implied in the introduction, we believe that other construction methods await discovery, and that possibly all seven point isospectral pairs will be constructable. By inference, this belief can be extended to all possible sets of isospectral graphs.

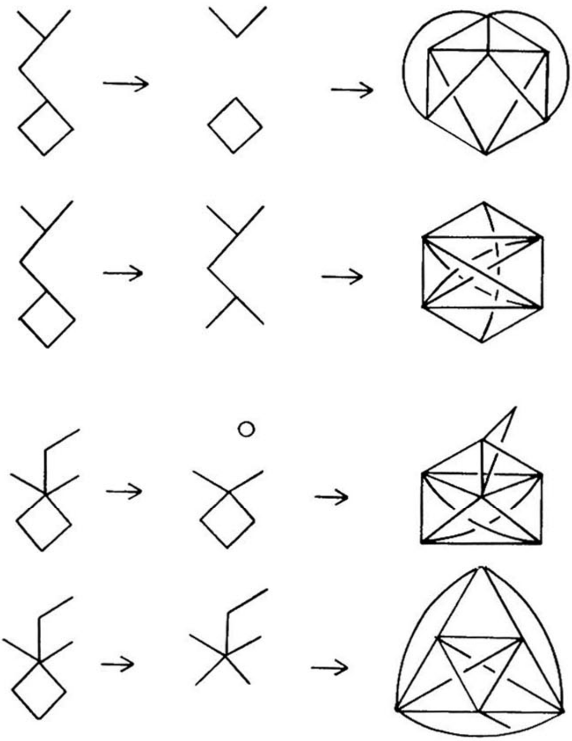


Fig. 12.5. Two pairs of 15-edge, seven-point isospectral graphs.

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