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ISOSPECTRAL POINTS AND EDGES IN GRAPH THEORY

John P. LOWE and Matthew W. DAVIS*
Department of Chemistry, 152 Davey Laboratory, Pennsylvania State University, University Park, PA 16802, USA

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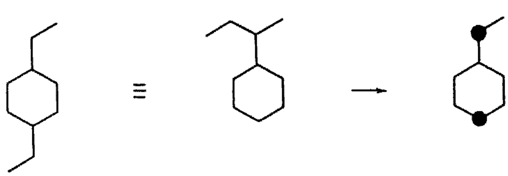
Abstract

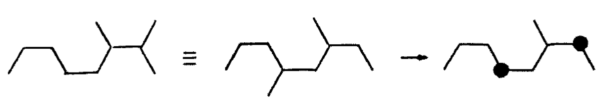
The relationship of isospectral points to symmetrically equivalent points in a graph is described. Many isospectral points are related to symmetrically equivalent vertices *via* an equivalence-preserving perturbation. A graph having isospectral *edges* is examined for clues to assist in finding other such graphs. Two families are found in this manner. Application of equivalence-preserving perturbations to edges that are initially symmetrically equivalent leads to an unlimited number of families of graphs, many with more than one pair of isospectral edges.

1. Introduction

It has been recognized for many years that nonisomorphic graphs can be isospectral [1,2], i.e. can have identical characteristic polynomial and roots (or eigenvalues). Frequently cited examples are **1a,b** and **2a,b**.



1a **1b** **1c**



2a **2b** **2c**

*Present address: Department of Chemistry, Massachusetts Institute of Technology, 77 Massachusetts Ave., Cambridge, MA 02139, USA

Graphs **1a** and **b** are isospectral and can be viewed as resulting from sequential substitution of a two-vertex fragment at the solid circles on graph **1c**. Similarly, the isospectral graphs **2a** and **2b** may be derived from sequential substitution of a single vertex at the solid circles in graph **2c**. Because of this, these solid-circle vertices are referred to as *isospectral points*. Generally, reversed sequential substitution of two distinct fragments at isospectral points generates isospectral graphs [2]. Thus, for example, **3a** and **b** are isospectral, where A and B are any two graphs.

3a **3b**

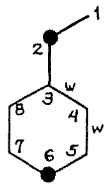
Examples of isospectral graphs that are *not* related through sequential substitution at isospectral points of a subgraph are known. **4a,b** is one such pair.

4a **4b**

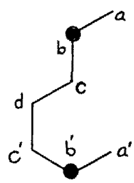
Studies of the nature of isospectral points [2–6] have led to the recognition that these points are *equivalent* in the mathematical sense of having coefficients of the same absolute value in each nondegenerate eigenvector (as well as in appropriately mixed degenerate eigenvectors), which is to say that these points behave in mathematical relations just as do points that are equivalent by symmetry. In both circumstances, perturbing the two sites in one way and then in the reversed way produces identical changes in energy, hence isospectral graphs. If the points are symmetrically equivalent, the two resulting graphs are identical, hence trivially isospectral. If the points are isospectral, the resulting graphs are different (nonisomorphic).

It has long been realized that adding a graph is not the only kind of change possible at isospectral points [2,3]. One can change the weight of such a vertex or of the edges connecting it to the rest of the graph.

In many cases, isospectral points are related to symmetrically equivalent points through an *equivalence-preserving perturbation* (EPP) of a continuous nature. For example, the isospectral points in **5a** remain equivalent for any value of the weight factor w at the indicated edges.



5a

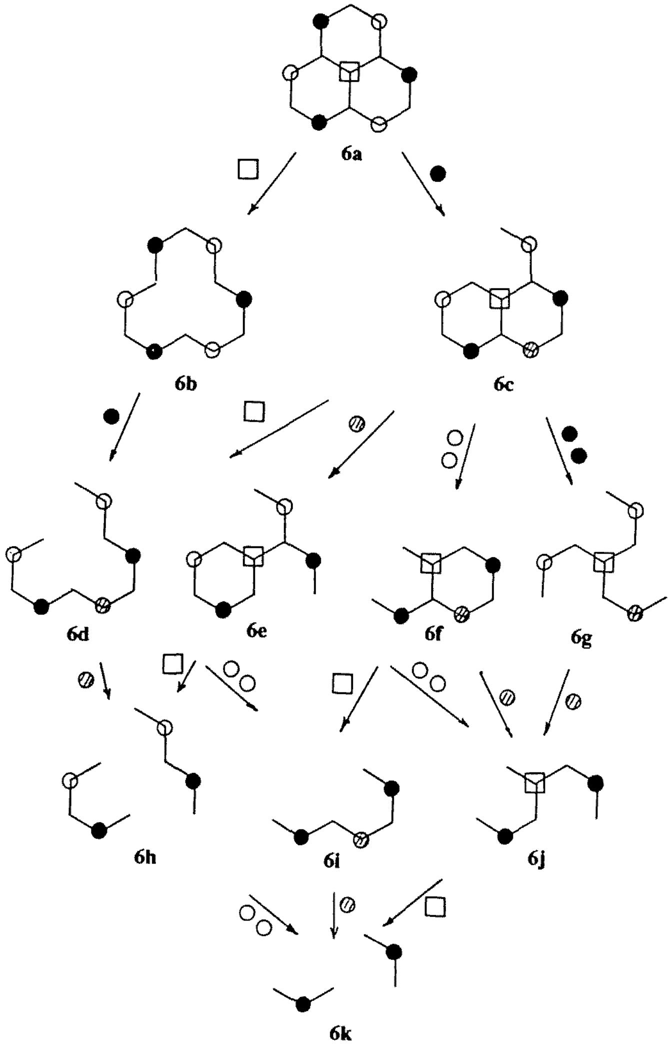


5b

When w equals zero, **5a** becomes **5b**, for which the isospectral points have become symmetrically equivalent. Thus, vertex 4 (or 8) of **5a** is a site where an EPP can occur. Such sites have been previously identified as *unrestricted substitution sites*. Herndon and Ellzey [3] point out that such sites have identical atom-atom polarizability indices with the two isospectral points. Hence, any perturbation there affects the isospectral points equally, preserving their equivalence.

The situation, then, is that when **5b** is identically perturbed at points a′ and c by adding a common vertex, the equivalence of a with a′ and also of c with c′ is lost, but that of b with b′ is preserved. Detailed perturbational analysis [5] has led to a general recipe for constructing additional graphs with isospectral points.

The above example shows how isospectral points may become symmetrical points in a *smaller* graph through an EPP at an unlimited substitution site. They may also become symmetrical through an EPP to a larger graph. Herndon and Ellzey [3] have shown that certain larger graphs having threefold symmetry contain subgraphs with isospectral points related by the symmetry of the parent. Building upon their ideas leads to **6a**–**6k** as an example of the graphs related by various EPPs taken in different orders. **6a** has two sets of vertices that are related by the C_3 operation, shown as filled and empty circles. This symmetry equivalence is not affected by removal of the central vertex (marked by a square), which means that we can remove this vertex initially, to give **6b**. Surprisingly, we can remove it later (after other changes) and it *still* has no effect on the symmetry equivalence of these two sets of vertices. A perturbation at a solid-circle vertex affects equally the other two solid vertices by symmetry [3], so substitution at or removal of a solid circle (to give **6c**) is an EPP. Interestingly, the hollow-circle sites symmetrically located about the EPP site (equal number of perimeter bonds on either side) undergo identical changes because of the symmetries of the eigenvectors, so their equivalence is preserved also. Not so the more distant hollow circle. It loses its equivalence to the others but, remarkably, becomes itself an EPP site for *both* sets of isospectral points. We mark it with a shaded circle. We have so far identified two EPP sites in **6c**, marked with a square and a shaded circle. There are two others that occur in groups. They are the isospectral pairs themselves [3,5]. Each *pair* is an EPP pair for the other pair of isospectral points. Thus, removal of the hollow circle pair from **6c** gives **6f**, in which the solid circles remain equivalent. The result of all this is that there are five EPP operations that can be applied to **6a** *in any order*. Some orders are such that the symmetric relations between points are always retained in an obvious way, e.g. **6a** → **6b** → **6d** → **6h**. Others produce



graphs having isospectral points, as in **6c**, **6e**, and **6f**. (Note that **6f** is **1c**, with a vertex substituted at the unlimited substitution site.)

6a is unusual in the number of EPP operations it permits. Not all threefold symmetric graphs are so rich. For example, **7** and **8** undergo only the first step (removal of a solid circle), to yield one pair of isospectral points and no other EPP sites. On the other hand, **9** behaves like **6a**. Detailed perturbational analysis similar to that in ref. [5] shows why this is so.

It is natural to ask whether all isospectral points are related to symmetrical points through EPP operations. Certain cases exist where we have not seen a relation to symmetry, for example **2c** and **10**. However, failure to find such connections is not proof that they do not exist.

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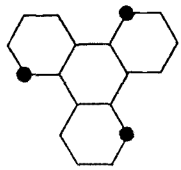

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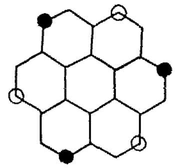

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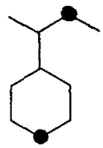

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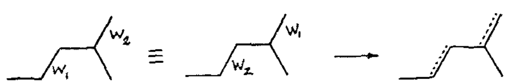
The current understanding, then, is that isospectral graphs are *sometimes* related through sequential perturbations at isospectral points in a common graph, and isospectral points are *sometimes* related to symmetrically equivalent points *via* an equivalence-preserving perturbation.

2. Isospectral edges

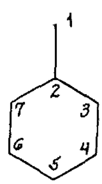
It has been noticed [7] that isospectral graphs can be produced by sequential alteration of edge weights, as in **11a,b**. The symbolic representation of the relation between **11a** and **b** is given by **11c**. Here, two edges that are not equivalent by symmetry



11a **11b** **11c**

nevertheless behave as if they are equivalent. We refer to them as isospectral edges [8] and indicate them with dotted lines.

A mathematical requirement for isospectral edges is that products of eigenvector coefficients at vertices attached by such edges be equal in every eigenvector for the graph (using proper zeroth-order combinations in degenerate cases). While this is a necessary requirement, it is not sufficient. Thus, **12** is a graph having equal products for



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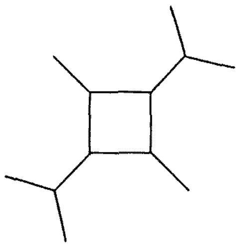
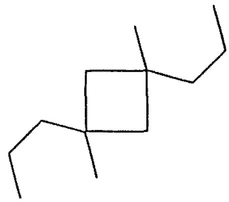
coefficients between vertices 1, 2 and 4, 5. Furthermore, vertex 3 is an EPP for these edges. However, the edges are not isospectral because changing $w_{1,2}$ affects the eigenvalues differently than equally changing $w_{4,5}$.

Isospectral edges permit the creation of isospectral polymers by creating links between such special vertices in *separate, identical* graphs. Joining one vertex of an isospectral edge to the other vertex in a second monomer and also joining the other pair of vertices creates a dimer graph that must be isospectral with that produced by the same procedure using the other isospectral edge. In this way, **13a,b** can be made from **11**. The process can be continued to trimers, etc.



13a



13b

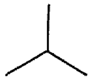
Graph **11** was the only one known by us to contain isospectral edges, and we wished to determine whether more cases exist and, if so, seek rules for finding them. One can take a "brute force" approach, seeking the proper coefficient product relation in randomly selected graphs. We have taken a more directed approach, checking promising generalizations of the situation represented by **11**.

One observation comes from setting w_1 and w_2 sequentially equal to zero in **11**. This gives **14a** and **14b**, which are isospectral graph *pairs*. This shows that **11** can be formed in two ways by joining collectively isospectral pairs of graphs through edges

14a

14b

that are isospectral. In one case we join two even-alternant graphs, in the other two odd-alternants. This odd–odd and even–even observation is helpful. A pair of odd-alternant graphs must have at least two null eigenvalues. This means that the pair of even-alternants must too. However, even-alternants with null eigenvalues are not common. (When an even-alternant has null eigenvalues, it will have an even number of them.) So, one is led to examining pairs of even-alternants where one member of the pair (e.g. **15**, **16**, **17**) has a degenerate null eigenlevel.



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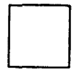

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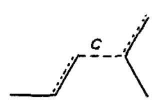
Other strategies suggest themselves. **14a** corresponds to attachment of a single vertex, which has a nonzero coefficient in the eigenvector for the null eigenvalue, to a site in the other fragment which has a *zero* coefficient in the eigenvector for the null eigenvalue. Again, the edge being created is one of the isospectral edges.

A third approach was suggested to us by the observation that the pair of null eigenvalues do not change value when the fragments are joined together. That is, while most eigenvalues change with changing the edge weight, the null values do not. Thus, **11a,b** have two null eigenvalues regardless of the values of w_1 and w_2. This suggests bringing together odd-alternant fragments so that the eigenvectors of the null eigenvalues will not interact, i.e. connecting a zero-coefficient vertex in one fragment with a nonzero-coefficient vertex in the other fragment. This is consistent with **14a**, but it permits, in addition, **18**. In this case, the new edge c is *not* one of the isospectral edges.



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These clues have led us to two classes of graphs with isospectral edges as well as two isolated examples. One class (fig. 1) may be regarded as resulting from addition of a vertex to the penultimate point of an n-membered, linear graph, where n is odd. We

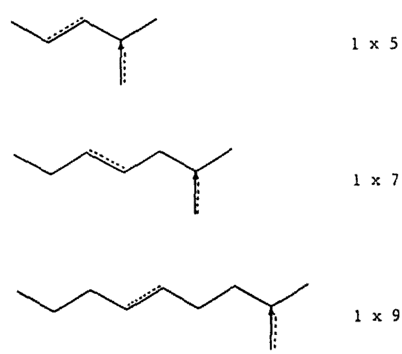
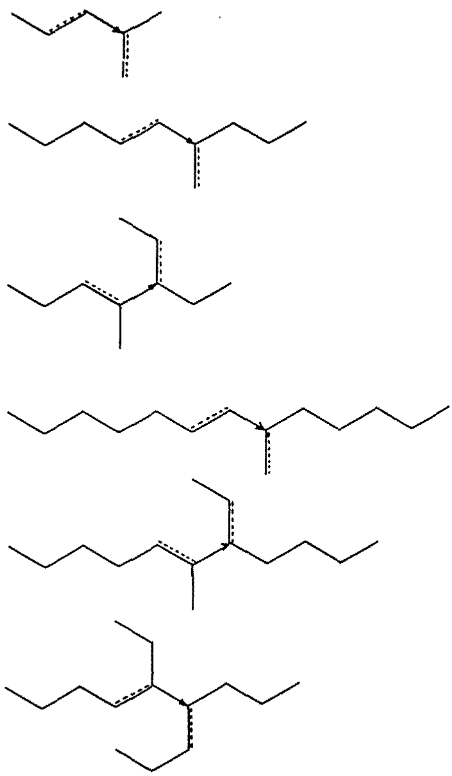


Fig. 1. The first three members of the $1 \times n$ family. Dotted edges are isospectral. Arrows indicate edges used to link subgraphs.

call this a $1 \times n$ process. The isospectral edges are the new edge and the edge connecting the central vertex of the n-chain to the vertex *away* from the end being altered. Graph **11** is the result of the 1×5 process and is the smallest member of this family. Connecting the lone vertex to other vertices of the n-chain does not produce analogous families of graphs with isospectral edges. The second class arises by application of the approach indicated in **18**. The first few members are shown in fig. 2. The graphs being



3 x 3 (1,2')

5 x 5 (1,2')

5 x 5 (2,3')

7 x 7 (1,2')

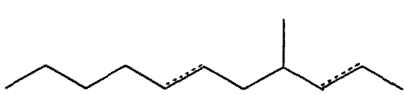
7 x 7 (2,3')

7 x 7 (3,4')

Fig. 2. The first three sets of $n \times n$ graphs containing isospectral edges. Dotted edges are isospectral. Arrows indicate edges used to link subgraphs.

joined in this method are identical, so the process is called $n \times n$. The vertices being joined are associated with different ends of equivalent edges in the two subgraphs. Thus, in 7×7, an end vertex in one graph links to the penultimate vertex in the other graph. The isospectral edges in the resulting graph are the ones that connect these vertices in the subgraphs. Here, we find that all appropriate vertex linkages lead to isospectral edges. Thus, 7×7 produces three graphs with isospectral edges, with can be labeled 1–2′, 2–3′, and 3–4′.

Two graphs which do not appear to be members of families are **19** and **20.**



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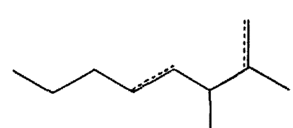

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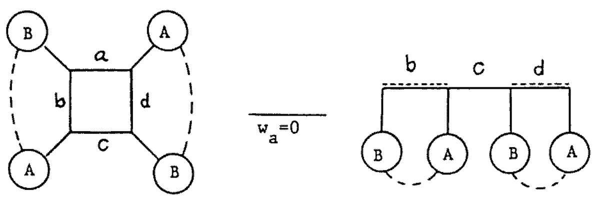
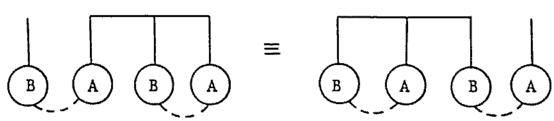
The edges indicated by arrows in fig. 2 are evidently EPP edges since the isospectral edges are identical in the separated subgraphs and equivalent when the subgraphs are joined. Thus, we can view the isospectral edges in the $n \times n$ family as being equivalent because of preserved "symmetry equivalence" (actually, a preserved "identity equivalence"). An EPP edge is not evident in the $1 \times n$ family (except for 1×5, which is 3×3).

Even though the $1 \times n$ family and **19** and **20** show no resolution to the identical subgraphs *via* edge removal, there may be an EPP relation to symmetry in each case to a graph with *more* edges. We approach this similarly to the way Herndon and Ellzey did for isospectral points [3], through the use of symmetry equivalence. Consider graph **21**, where dashed lines indicate optional edges, and A,B are any graph fragments. If the



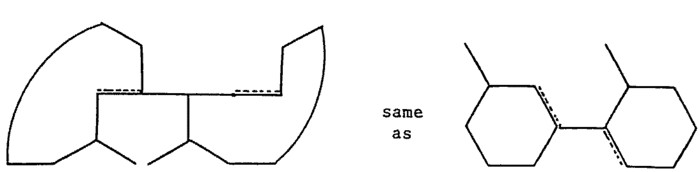
21 **22**

weight of edge a is set equal to zero, graph **22** results. Edges b and d become the isospectral pair shown. Edge c becomes an EPP edge, as is most easily seen by imagining its weight to go to zero. If isospectral edges b and d are sequentially given zero weight, we obtain the isospectral graphs **23a,b**. If the optional edges are not present,



23a **23b**

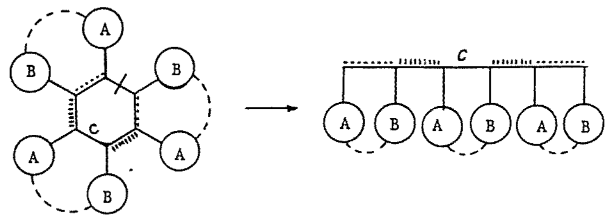
and if A and B are straight-chain graphs, **22** generates all the $n \times n$ cases. For example, if A is one vertex and B is two, **22** becomes $5 \times 5(2,3')$. If A has four vertices and B has two, and the optional edges connecting A and B are used as shown in **24**, we obtain



24 **24**

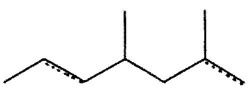
rings with isospectral edges. Clearly, **22** cannot give us the family of fig. 1 or graphs **19** or **20** because it must always produce isospectral edges with one intervening edge.

The six-membered ring with substituents offers more possibilities (**25** → **26**). Here, we obtain two sets of isospectral edges, one set with a single intervening edge, the other set with three intervening edges. Edge *c* is not an EPP edge in this case. The

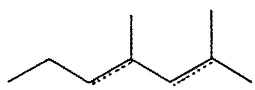


25 **26**

simplest case results when *A* is a vertex, *B* is nothing, and the optional bonds are absent. This gives **27a,b** (the same graph with the different isospectral edges indicated). An



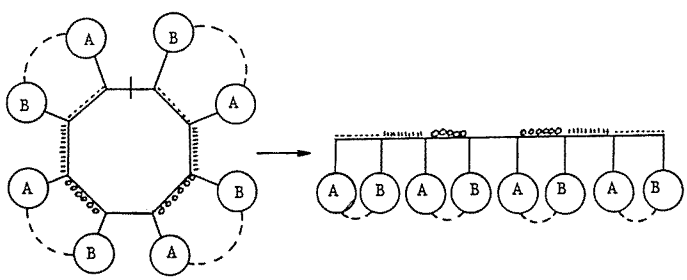
27a



27b

unlimited number of graphs with isospectral edges separated by three edges can be generated from **26**, but none of them correspond to **19**, **20** or fig. 1.

On can continue this approach with larger cycles, as in **28**. Here, there are three pairs of isospectral edges.



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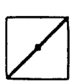
Formation of isospectral edges is prevented in cycles where connections exist between the various subsections, as in **29**–**32**.



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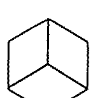

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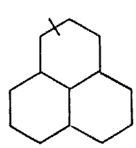

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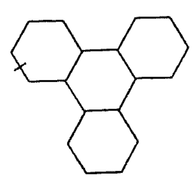

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3. Conclusions

Isospectral points are similar to symmetrical points in their mathematical properties. In many cases, they can be shown to *become* symmetrical by a transformation (the "growing in" or "fading out" of one or more vertices) which affects both points identically and hence preserves their equivalence. Isospectral edges are similar in this respect. Here, we have shown that symmetrical edges can become asymmetrical, without becoming inequivalent, through the growing in or fading out of another edge. (The growing or fading edge is the analogue of the unrestricted substitution site, and might be called an unrestricted-order edge.) Use of this transformation allows the generation of an unlimited number of families of graphs having one or more pairs of isospectral edges.

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[8] Comparison of **11a** and **5a** shows that *edge* weights are also involved when a *vertex* is removed from a graph. The distinction is that removal of a vertex amounts to setting the weight factor to zero for *both* associated edges.