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ISOSPECTRAL GRAPHS, SYMMETRY, AND PERTURBATION THEORY

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ABSTRACT

Isospectral sets of points in graphs are equivalent in the same manner as are symmetry-equivalent sets of points. This allows us to transfer observations concerning relations between symmetry-equivalent points to less-obvious equivalent but unsymmetrical points. The equivalence of isospectral points in a graph can sometimes be understood to result from a symmetrical equivalence in a simpler graph. The change to the more complex graph destroys the symmetry but does not destroy the equivalence between the points. All the points in a pair of isospectral graphs are members of isospectral sets. Arguments based on perturbation theory are used to expose these relationships.

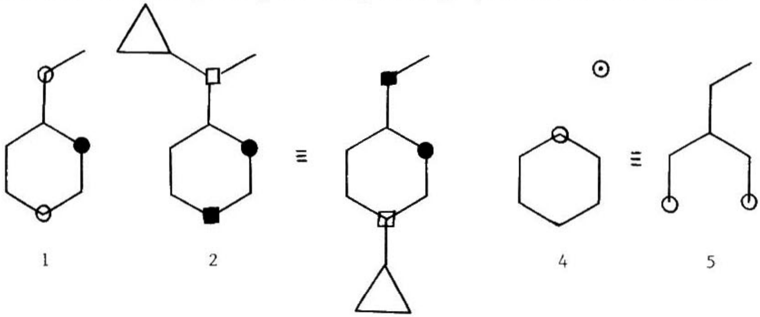
I. INTRODUCTION

Isospectral graphs and molecules have been recognized to exist for more than twenty-five years.[1-5] A graph is a collection of points (vertices) connected by lines (edges).[6-8] The adjacency matrix for a graph is constructed by numbering each vertex of the graph and placing a one in each row-column position of the matrix for which an edge exists, otherwise a zero. The adjacency matrix for a graph is therefore constructed in the same manner as is the topological matrix in simple Huckel theory. An adjacency matrix is associated with a characteristic polynomial and a set of eigenvalues. It was once thought that the polynomial and set of eigenvalues for a graph might be unique, providing a convenient "fingerprint" for purposes of storage of data on molecules, but it has since been found that nonidentical graphs can have the same polynomial and set of eigenvalues.[1-5,9-17] Such graphs are isospectral. Molecular graphs are those representing realistic molecular structures (i.e., not too many edges connected to a single vertex), and when such graphs are isospectral, one speaks of isospectral molecules.

An important series of papers[9-22] shows how one can use certain special vertices in graphs to construct unlimited numbers of isospectral graphs. Herndon and Ellzey[13] and Zivkovic, Trinajstic and Randic[12] point out certain relations which hold between the eigenvector coefficients at these special points. A subsequent article by D'Amato, Gimarc, and Trinajstic[18] discusses similar concepts in the context of special pairs of vertices. Our purpose is to generalize and extend the ideas presented in these papers and to answer some questions raised by D'Amato et al.[18]

II. DEFINITIONS AND EXAMPLES

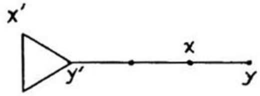
Graph 1 contains isospectral points (open circles), which means that the two nonidentical graphs resulting from substituting a structure at one point and again at the other are isospectral. Thus 2 and 3 are isospectral. Removal of isospectral points can be considered as a type of substitution. Thus 4 and 5 are isospectral graphs. Let us refer to the



1 2 3 4 5

open-circled sites in 1 as linked isospectral points, linked because they occur in the same graph. Isospectral graphs 4 and 5 have another interesting property: They each possess a pair of vertices (circled) which, when joined to a common vertex, result in two new molecules which continue to be isospectral. Thus 2 and 3 result from 4 and 5 respectively by substitution of a four-vertex graph. 1 is the result of substituting a single vertex into 4 or 5; thus there can be cases where substituting into graphs like 4 and 5 produces one graph rather than two isospectral graphs. Let us refer to the open-circled sets in 4 and 5 as unlinked isospectral pairs (unlinked because each pair occurs in a different graph). (Randic[19] has proposed the term endospectral for linked isospectral points.)

Graph 6 contains linked isospectral pairs. One pair is labeled x,x', the other y,y'. (Either of the equivalent corners of the triangle could be taken as an x' site.) Therefore, graphs 7 and 8, which result from bridging x,x' and y,y' respectively with a single vertex v, are isospectral. (Removal of the x,x' pair from Graph 6 results in a graph which is not isospectral with the graph produced by removal of the y,y' pair.) A vertex which connects an isospectral pair, like those indicated



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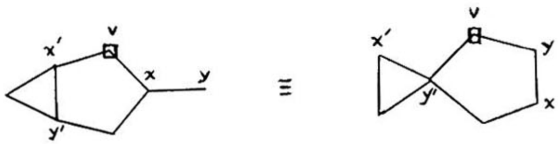
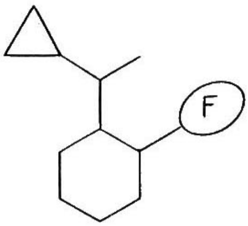


7 8

as open squares in 2, 3, 7, and 8, is called a bridging vertex.

Graph 1 contains also an unrestricted substitution point (solid circle) which means that substituting any fragment at this site does not destroy the isospectral relation of the sites marked by open circles. As a result, 9 and 10 are isospectral. We can view these as resulting from attaching an arbitrary fragment F to the unrestricted substitution point in 1, followed by substitution at the linked isospectral points on the resulting graph, or we can view them as resulting from first forming 2 and

3, and then attaching F to the solid-circle site on each of these graphs. Viewed in the latter manner, the solid-circle sites in 2 and 3 are unlinked isospectral points, or substitution partners. Observe that removal of these points from 2 and 3 results in formation of the same graph. (Each of these solid-circle points in 1-3 has an equivalent point related through the two-fold symmetry of the graph.)



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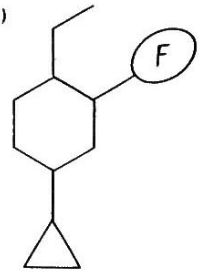

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III. EARLIER OBSERVATIONS, FORECAST OF CONCLUSIONS

Herndon and Ellzey[13] showed that "isospectral points must have identical absolute values of eigenvectors in every nondegenerate eigenlevel," and also that the sum-over-degenerate-eigenvalues of squares of coefficients at isospectral points must be equal. D'Amato, et al.[18] conjectured that, in linked isospectral pairs, "the sum of coefficients at the x-marked vertices is equal to the sum in the y-marked vertices" in each eigenvector, and also that "the bridging vertices serve as substitution partners for the graphs" 7 and 8.

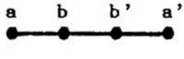
We show here how perturbation theory treats these aspects of graph theory and reveals some previously unrecognized relations. Specifically, we show that:

1) An absolute value sum rule holds for isospectral pairs in nondegenerate eigenvectors.

2) The same absolute value sum rule holds for sets of degenerate eigenvalues, both for isospectral points or for isospectral pairs, if proper zeroth-order eigenvectors are used.
3) D'Amato's conjecture concerning bridging vertices is true in general.
4) The set of all points not included in the sets of isospectral points or pairs itself has interesting properties related to isospectrality.
5) Isospectral points or pairs are equivalent in effectively in the same manner as are symmetrically equivalent points, and sometimes this results from a preservation of equivalence when the symmetry of a molecule is destroyed by substitution.

IV. COEFFICIENT RELATIONS

The profusion of isospectral points, or pairs of points, linked or unlinked is greatly simplified by the realization that isospectral points (or pairs) are equivalent to each other in much the same manner as points that are equivalent by symmetry. Consider Graph 11. The points a and a' are equivalent to each other by symmetry, as are b and b'. Substitution



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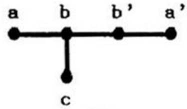

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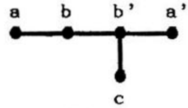

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of a vertex at b gives 12. Substitution at b' gives 13 which is obviously the same graph, hence trivially isospectral. We will argue that this situation is analogous to substitution at the isospectral points in 1, which yields nonidentical graphs but identical eigenvalues, or nontrivial isospectrality.

Let us look more closely at the way in which substitution at b and b' of 11 manages to produce the same set of new eigenvalues. Perturbation theory[23] yields expressions for the corrections to eigenvalues and eigenvectors in terms of the unperturbed eigenvalues and eigenvectors. The perturbation producing 12 is symbolized in 14: An interaction between an isolated vertex and vertex b is turned on. All contributions to the

14a 14b

changes in eigenvalues, and all coefficients for corrections to the eigenvectors depend *only* on the following: Eigenvalue and eigenvector coefficient for c, eigenvalues for 11, eigenvector values for 11 at point b. Clearly, the only ones of these variables that can change when we attach at b' instead of b are the eigenvector values for 11. Indeed, the eigenvector values *do* change because, in some eigenvectors, b and b' have coefficients of opposite sign. However, since we know that the eigenvalues are the same after either substitution, we know that the perturbational expressions for the eigenvalues must depend on absolute values of coefficients rather than algebraic values.

For a specific example of this, the second-order correction to the i-th eigenvalue is:

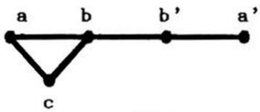
$$W_i^{(2)} = \sum_{j \neq i} \frac{\langle \phi_i | H' | \phi_j \rangle \langle \phi_j | H' | \phi_i \rangle}{\varepsilon_i - \varepsilon_j} \qquad (1)$$

where ε and ϕ are eigenvalues and eigenvectors, respectively, for Graph 14a and where H' is $\delta_{c,b}$, a Kronecker delta which permits vertex c to interact only with vertex b. If we let ε_c represent the eigenvalue associated with the isolated point c, and let b_i be the coefficient at vertex b in eigenvector ϕ_i, then it follows that (assuming $\varepsilon_c \neq \varepsilon_i$ and recognizing that the coefficient for vertex c is unity in ϕ_c)

$$W_i^{(2)} = \frac{b_i^2}{\varepsilon_i - \varepsilon_c} \tag{2}$$

i.e., that the second-order corrections to the eigenvalues depend on the absolute values of the coefficients at the site of attachment.

The recognition by Herndon and Ellzey[13] that "isospectral points must have identical absolute values of eigenvectors in every nondegenerate level" resulted from their perceiving the similarity of isospectral points and points equivalent by symmetry. We propose that isospectral pairs of points, like those in Graph 6, or in 4 and 5, likewise behave as symmetrically equivalent pairs of points, like the pairs a, b, and a', b' in 11. Obviously, bridging a, b in 11 gives the same graph as does bridging a', b':



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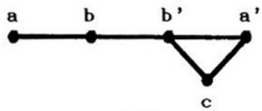


15b

The perturbation operator for the former process is $\delta_{ca} + \delta_{cb}$, leading to a second-order expression for the eigenvalue corrections of

$$W_i^{(2)} = \frac{(a_i+b_i)^2}{\varepsilon_i - \varepsilon_c} \tag{3}$$

Evidently, the fact that we get the same eigenvalues regardless of whether we bridge a and b or a' and b' of 11 results (at least to second order) from the fact that $(a_i+b_i)^2=(a'_i+b'_i)^2$.

Examination of higher terms in perturbation theory shows that sums of products of sums over two eigenvectors arise of the form

$$\frac{(a_i+b_i)(a_j+b_j)}{(\varepsilon_i-\varepsilon_c)(\varepsilon_j-\varepsilon_c)} \qquad (4)$$

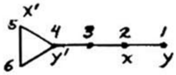
and that the absolute value of such products must remain unchanged when a and b are replaced by a' and b' if the eigenvalues are to be the same. In short, the points a and b are equivalent in concert to the points a' and b'. For Graph 11 this is obviously true, since a and a', and b and b' are individually equivalent. For Graph 6, on the other hand, the individual point x is not equivalent to y or to y'. It is not difficult to show that, for a case like 11, where the individual members of the sets are equivalent, there is an equality between absolute values of coefficient products in each nondegenerate eigenvector, viz.

$$|a_i b_i| = |a'_i b'_i| \qquad (5)$$

whereas such a relation does not exist for cases like 6.

The above findings require that the conjecture of D'Amato et al.[18] be modified to state that the absolute sum of coefficients at the x-marked vertices equals the absolute sum of coefficients at the y-marked vertices. Examination of the eigenvector list for 6 (Table I) shows that this requirement is met for all the eigenvectors except the degenerate pair at $\varepsilon = -1.000$. D'Amato et al. based their sum-rule on a coefficient analysis of Graph 6 which yields the relation:

$$(x+x')(1+\varepsilon) = (y+y')(1+\varepsilon) \qquad (6)$$

TABLE I. Eigenvalues and Eigenvectors for Graph 6. 

Vertex	ε=2.228	ε=1.360	ε=0.186	ε=-1.000	ε=-1.000	ε=-1.775
1(y)	0.090	0.485	-0.632	0.535	0.000	0.267
2(x)	0.201	0.660	-0.118	-0.535	0.000	-0.474
3	0.357	0.413	0.610	0.000	0.000	0.574
4(y')	0.595	-0.099	0.231	0.535	0.000	-0.545
5(x')	0.485	-0.273	-0.284	-0.267	0.707	0.196
6	0.485	-0.273	-0.284	-0.267	-0.707	0.196

TABLE II. Proper Zeroth-Order Eigenvectors for Bridging x points of Graph 6.

Vertex	x bridge	
1 (y)	-0.354	-0.401
2 (x)	0.354	0.401
3	0.000	0.000
4 (y')	-0.354	-0.401
5 (x')	-0.354	0.668
6	0.707	-0.267
v	0.000	*0.000

They argued that the sum of coefficients over x,x' points must equal that over y,y' points. However, another possibility is that $1+\varepsilon$ vanishes, which is indeed the situation which pertains for the degenerate eigenvectors at $\varepsilon=-1.000$. Nevertheless, because these points are isospectral pairs, our perturbation expressions lead us to expect that these coefficients still manage to satisfy the absolute sum rule. That is, we expect

$$|x_i+x'_i+x_j+x'_j| = |y_i+y'_i+y_j+y'_j| \qquad (7)$$

where i and j now refer to the degenerate levels, and where we have combined these degenerate level terms since their denominators always involve identical ε values. However, the numbers in Table I do not satisfy this relation. The resolution of this problem comes from realizing that a perturbational treatment over degenerate eigenvalues requires use of proper zeroth-order eigenvectors. The proper eigenvectors, $\phi^{(0)}$, must satisfy the requirement

$$\langle\phi_i^{(0)}|H'|\phi_j^{(0)}\rangle = 0 \quad . \qquad (8)$$

Since we are comparing two different perturbations (H'_x and H'_y) we must anticipate two different sets of proper zeroth-order eigenvectors.

Equation 8 leads to the following relation for H_x':

$$(x_i^{(0)} + x'^{(0)}_i)v_j^{(0)} + (x_j^{(0)}+x'^{(0)}_j)v_i^{(0)} = 0 \qquad (9)$$

An analogous expression applies for Hy'. Here i and j continue to refer to degenerate eigenvectors and v refers to the coefficient at the bridging vertex which is becoming attached to points x, x' or y,y'. One's first reaction is to expect $v^{(0)}$ to be zero in $\phi_i^{(0)}$ and $\phi_j^{(0)}$. Indeed, v doesn't even appear in Table I. But we are really concerned with the nature of ϕ_i and ϕ_j <u>in the limit</u> that H' goes to zero, and so equation 9 is only useful in the context of H'_x not being exactly zero, hence $v^{(0)}_i$ or $v^{(0)}_j$ not necessarily being exactly zero. There are various ways to satisfy Equation 9. Some of them are:

Case 1. $v_i^{(0)} = v_j^{(0)} = 0$

Case 2. $x_i^{(0)} + x'_i{}^{(0)} = 0,\ v_i^{(0)} = 0$

Case 3. $x_i^{(0)} + x'_i{}^{(0)} = x_j^{(0)} + x'_j{}^{(0)} = 0$

Case 4. $x_i^{(0)} + x'_i{}^{(0)} = x_j^{(0)} + x'_j{}^{(0)} \neq 0,\ v_i^{(0)} = -v_j^{(0)} \neq 0$

Case 1 corresponds to the situation where neither of the eigenlevels is influenced by the perturbation. This implies that, in each eigenlevel, sites being bridged are "nonbonding" with respect to the bridging vertex, i.e., that

$$x_i^{(0)} + x'_i{}^{(0)} = 0 \text{ if } v_i^{(0)} = 0,$$

and similarly for j bridging. This reveals that Case 3 is identical to Case 1. Case 2 corresponds to a situation where only one of the two eigenlevels is unperturbed by the bridging vertex. Case 4 corresponds to a situation where the degenerate levels are perturbed in opposite directions.

Case 2 is satisfied by the degenerate eigenvectors in Table I for the perturbation H'_y, since the sum of coefficients in one of the eigenvectors over the y points is zero. Thus, we anticipate that Graph 8 will continue to possess one eigenvalue at $\varepsilon = -1.000$, and this turns out to be true.

The proper zeroth-order eigenvectors for H'_x appear in Table II. Again, Case 2 is the one which is satisfied, which is necessary since the result of H'_x must be the same as H'_y if the new molecules are to be isospectral, and we have seen that only one of the degenerate eigenvalues is shifted by H'_y.

The absolute sum rule is now satisfied since, from Tables I and II and Equation 7:

$$|0.354-0.354 + 0.401 + 0.668| = |0.000 + 0.000 + 0.535 + 0.535| \qquad (10)$$

It even holds for each eigenvector individually since the absolute sum of the first pair of coefficients on the left agrees with that for the first pair on the right, and likewise for the second pairs.

Thus, isospectral pairs display the same coefficient relationships as do pairs of points related by symmetry, just as do isospectral points with symmetrical points (with one difference: isospectral pairs, when separated and compared as individual points, need not retain the isospectral relation.) This means that we can look for and prove various relationships concerning isospectral points or pairs by appeal to symmetric analogs. In other words, isospectral points can be regarded as being related by a kind of "hidden symmetry." It results, as Randic[24] has shown, from the fact that isospectral points are equally connected to all other points in their graphs, as measured by self-returning walks. Symmetrical points are obviously equally connected; isospectral points are also equally connected, but not so obviously. Symmetric pairs are equally connected individually and, hence, in concert. Isospectral pairs are equally connected in concert, but not necessarily individually. Since it is the degree of connectedness which is the fundamental property governing eigenvalues, we see that symmetrically related points or pairs of points are a subset of the set of points equally connected to their graphs.

(Before moving to the next point, we should note that Equation 10 holds with or without the absolute value signs, so after all, there is no eigenvector for Graph 6 that disobeys the more restrictive sum-rule of D'Amato et al.[18] However, other examples exist where the more restrictive sum rule fails. One such case appears in Table III of D'Amato et al.[18] for $\varepsilon=1.000$. It is possible to show, from perturbative arguments, that equivalent points a and a' must disagree in coefficient sign in at least one eigenvector, or else that there must be a degeneracy so that different zeroth-order eigenvectors can apply to different perturbations. For if this were not the case, and we perturbed at site a, corrections made to each eigenvector at points a and a' would be identical. But we know that this is not the familiar result. The eigenvectors of the new graph are different in value at the points a and a'. The system is able to tell which site is being perturbed and which is not and to respond differently at the two sites. But it cannot do so unless at least one eigenvector is different at a and a'.)

V. IDENTICAL POINTS AND EQUIVALENT POINTS

We see that there is a close connection between substituting serially at symmetrically equivalent points, as in 11-13, and substituting serially at isospectral points, as in 1-3. In each kind of case, all of the eigenvalues and absolute eigenvector coefficients at the two points are identical so that, to infinite order in perturbation theory, the points are equivalent.

Now we come to a subtle but important observation. In the case of symmetric substitutions, we produce identical graphs, like 12 and 13. This means that the added vertex, c, is identical in 12 and 13. Likewise for c in 15a and 15b. However, if a vertex is serially substituted to the isospectral points in 1, nonidentical graphs result and the added vertex is not identical in the two new graphs. Likewise, v in 7 is not identical to v in 8. However, even though these added vertices are not identical, they are equivalent. To see this, we reverse our point of view and consider 6→7 to be a perturbation of v by points x and x' of 6. The resulting eigenvector coefficients of v in 7 are determined by absolute sums of coefficients at x and x', the coefficient at v, eigenvalues of 6 and of v. The process 6→8 differs only in that the absolute sums of coefficients for y and y' replace these for x and x'. But these absolute sums are the same, so the resulting coefficients for v in 8 must have the same absolute values as those for v in 7. Since the eigenvalues for 7 and 8 are also identical, it follows that v in 7 and v in 8 are equivalent, hence unlinked isospectral points, (or substitution partners). This proves one of the conjectures of D'Amato et al.[18]

A similar argument holds for the isospectral points themselves. That is, b of 12 is identical to b' of 13, so the open-square vertex in 2 is equivalent to that in 3, which means that they are unlinked isospectral sites. Likewise, the unused isospectral points, b' in 12 and b in 13, are identical, and so the solid-square points in 2 and 3 are equivalent. These reciprocal equivalence rules were pointed out by Herndon and Ellzey.[13]

VI. GROUPS OF POINTS

We have argued above that points which become identical in symmetric-substitution cases become equivalent in isospectral-substitution cases. This can be extended to groups of points: Whereas a, b in 15a are identical to a', b' in 15b, x, x' in 7 are equivalent to y, y' in 8. In other words, isospectral (equivalent) pairs which have been directly perturbed by bridging remain isospectral (equivalent) in the new molecules. The isospectral pairs not directly perturbed behave similarly: a', b' in 15a are identical to a, b in 15b, y, y' in 7 are equivalent to x, x' in 8. Finally, all the remaining points (spectator points) constitute a group which is identical for symmetric cases, equivalent for isospectral cases. Thus, the unlabeled points in 7 and 8 are equivalent pairs, or unlinked isospectral pairs.

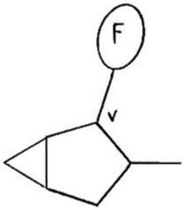
As a result of the above observations we see that, when two isospectral graphs are created from an initial graph by serial substitution, every point in each graph belongs to a group which equivalent to a group in the other graph. Since combinations of equivalent groups remain equivalent, it follows that the group of all points in one graph is equivalent to all the points in the other.

We have been discussing two kinds of equivalent point or group of points--those equivalent by symmetry (hence also by connectivity) and those equivalent by connectivity but not by symmetry. We will henceforth use the term symequivalent for the first class and conequivalent for the second. Conequivalent points are isospectral points.

VII. SOME EXAMPLES

Consider 6. Bridging x,x' points and y,y' points serially gives isospectral graphs 7 and 8. The bridging vertices are labeled v.

1. The sites v are conequivalent (hence unlinked isospectral points):



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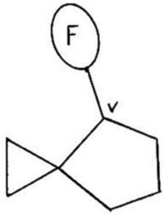

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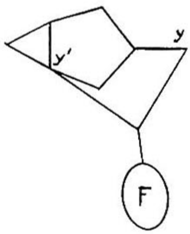
2. The pair y, y' in 7 is conequivalent with the pair x,x' in 8 (hence unlinked isospectral pairs):



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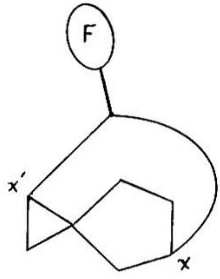

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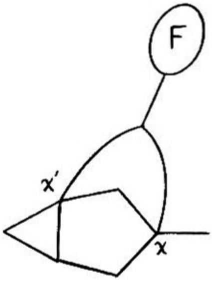
[Randic has pointed out (personal communication) that, if the connection is made by a simple bridging vertex, the resulting graphs are identical.]

3. The pair x, x' in 7 is conequivalent with the pair y, y' in 8:



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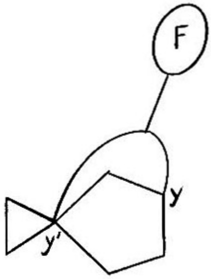

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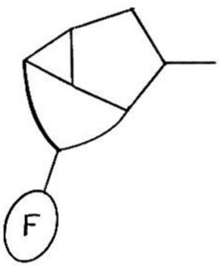
4. The spectator points, unlabeled in 7 and 8 are conequivalent pairs:



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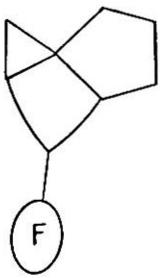

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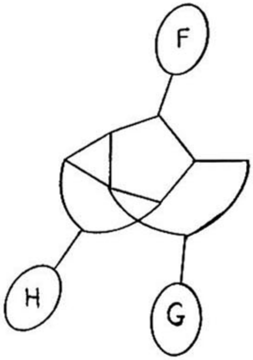
5. Any combination of conequivalent groups retains conequivalence:



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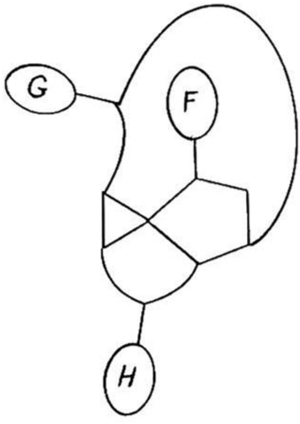

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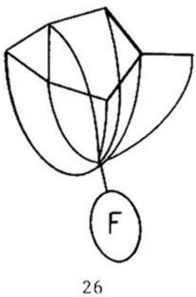

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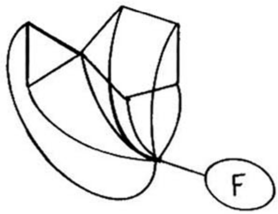

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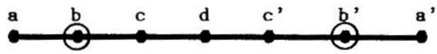
The fact that 7 and 8 possess symmetry means that there are some equivalences present within the groups mentioned above. Clearly, there are two locations in each graph that could be labeled v, for instance. This symequivalence allows separation of the spectator pair into <u>individual</u> equivalent points in this pair of graphs. This means that each of the unlabeled points in 6 is individually an unrestricted substitution point.

VIII. PRESERVATION OF EQUIVALENCE

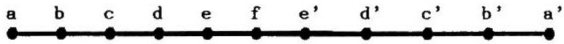
Where do linked conequivalent points or groups of points like those in 1 or 6 "come from?" We find that they are sometimes points which are symequivalent in a graph produced by annihilation of an unrestricted substitution point.[25] For example, removal of the solid-circle vertex in 1 gives Graph 28 in which the open-circle vertices are symequivalent. In



28

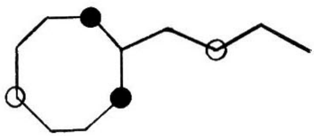
other words, linking points a and c' of 28 with a new vertex preserves the equivalence of b, b', but not that of a with a' or c with c'. One might guess that it is simply the fact that the set b,b' is the only equivalent set not directly involved in the perturbation that is responsible, but this is not correct. Adding two more points to form a nine-point chain does not produce a second pair of conequivalent points after the analogous substitution. In fact, no conequivalent points survive in that case. Detailed consideration of perturbation terms for the transformation of 28 to 1 (see Appendix) reveals that b,b' equivalence is preserved because 28 has a central point bridging two odd-membered subchains, because the linkage between a and c' is between points which are symequivalent to vertices a and c which are in turn symequivalent within the subchains, and because b,b' are in the center of the subchains. These factors combine to prevent the perturbational mixing of eigenvectors from changing the absolute coefficients at b differently from those at b'. (Since none of these factors involves the eigenvalues or coefficients for the bridging vertex, bridging vertex •—(F) can be used, which means that the vertex is an unrestricted substitution point.)

Recognizing these factors enables us to produce new cases. The next-larger linear graph from which we can build in the analogous manner is 29. We expect points c and c' to remain equivalent for cases where



29

a new vertex bridges a,e' or b,d' (or both at once). Thus, the open circles in 30 and 31 are conequivalent, or isospectral points. The solid circles are unrestricted substitution points.



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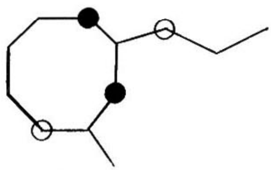

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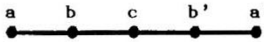
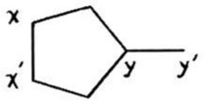
The relation of isospectral (conequivalent) pairs to symequivalent pairs is likewise of interest. Consider 32. Clearly the pair of



32

points a,b is symequivalent to a',b', and pair a,b' is symequivalent to a',b. If 32 is bridged at a,b, we obtain 6, so we know that equivalence between a,b' and a',b is retained. If we bridge 32 between a and b', we obtain 33. This graph is known to have isospectral pairs x,x' and y,y'



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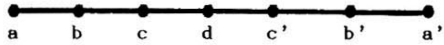
which means that the equivalence retained in this case is that between a,b and a',b'. In each case we retain equivalence between pairs wherein one point is involved in bridging and the other is not.

A perturbational analysis of 32 (Appendix) reveals the conditions which give rise to preservation of pair equivalence. The results are rather simple and are best explained using examples. Consider graph 32. The fact that certain symequivalent pairs retain equivalence when that graph is perturbed by linking a,b or a,b' rests on the facts that (1) a symmetry plane exists which cuts through a vertex (c) but does not bisect any edges, and (2) the points a and b are symequivalent in "their part" of the graph (all points outside and on one side of the reflection plane). (This means, of course, that a',b' must also be symequivalent in their part.) Consider graph 11. Linking a,b or a,b' does not maintain equivalent pairs. This results from the fact that the relevant symmetry plane bisects an edge.

Given this rather simple prescription, one can quickly create innumerable graphs having isospectral pairs of sites. Obviously, any odd-numbered chain is a candidate. 34 can be linked at



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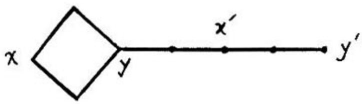
a,c to retain equivalence of a+c' with c+a' (see 35). Linking a,c' retains equivalence of a+c with a'+c' (36). But 36 is the same as 1: The bridging



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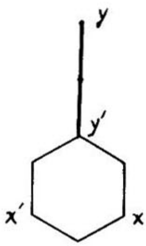

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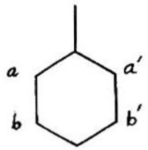
of 34 to produce 36 simultaneously meets our requirements for making b and b' into isospectral points and those for making a,c and a'c' into isospectral pairs. Note that bridging a,b of 34 does not work because a and b are not symequivalent in their "part" of the graph.

Graph 37 is a nonlinear case that meets the stated conditions. The plane cuts the three unlabeled vertices, and a is symequivalent with b



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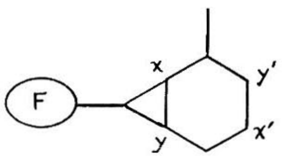

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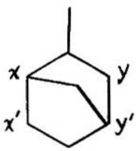

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in its fragment. As a result, bridging a and b to give 38 leaves the pair a,b' equivalent to a',b, whereas bridging a and b' to give 39 makes a,b equivalent to a',b'. (The bridging vertex is an unrestricted substitution site in all these cases, as explicitly indicated in 38.)

Graph 33 does not work in the same manner because the symmetry plane bisects a bond.

IX. CONCLUSIONS

Isospectral points or groups of points, linked or unlinked, are equivalent to each other in the same operational manner as points or groups of points that are equivalent by symmetry; the absolute values of coefficients (summed over groups) in all eigenvectors, including proper zeroth-order degenerate cases, are the same and the eigenvalues are the same. This means that classes of points or groups of points which become identical in symmetry-substitution cases become equivalent in isospectral-substitution cases. It appears that the existence of linked isospectral points or groups of points can sometimes be attributed to preservation of symmetric equivalence existing in a related graph.

Appendix

Perturbational Analysis of Preservation of Equivalence

I. Preservation of Equivalence Between Two Sites.

Consider a seven-vertex linear graph, <u>28</u>, with eigenvectors and eigenvalues as indicated in Fig. 1. Let the coefficient for vertex c' in eigenvector ϕ_i be symbolized by c'_i. By symmetry, a is equivalent to a', b to b' and c to c'. We have noted earlier that bridging this graph between c and a', as in <u>1</u>, destroys the equivalence of a with a' and c with c' but does not destroy the equivalence of b with b'.

When the perturbation due to bridging occurs, the eigenvectors on the seven original vertices undergo changes which are expressible entirely in terms of mixing among the original eigenvectors. That is, the original eigenvector ϕ_i becomes some new eigenvector, ϕ'_i which can be written as $\phi'_i = \phi_i + \lambda_{ji}\phi_j + \lambda_{kj}\phi_k + \ldots$ (Inclusion of coefficients from the bridging graph and renormalization would be required for complete expression of ϕ'_i, but that is not of concern here.)

In order for the vertices b and b' to remain equivalent, it is necessary that, for each eigenvector ϕ_i, any change in the absolute value of b_i be equalled by the change in absolute value of b'_i. That is

$$\left| b_i + \sum_{j \neq i} \lambda_{ji} b_j \right| = \left| b'_i + \sum_{j \neq i} \lambda_{ji} b'_j \right|$$

There are some features of the eigenvectors in Fig. 1 that can help in our analysis: Each eigenvector is either symmetric or antisymmetric for reflection through the central vertex, giving rise to the labels S and A in Fig. 1. Since the reflection plane cuts a vertex, it follows that each antisymmetric eigenvector is symmetric or antisymmetric within each subchain. (This follows from the analytical expression for such eigenvector coefficients,[12] and is not true for linear graphs with an even number of centers, where the plane must bisect an edge.) This symmetry condition is indicated by the subscript labels s and a in Fig. 1.

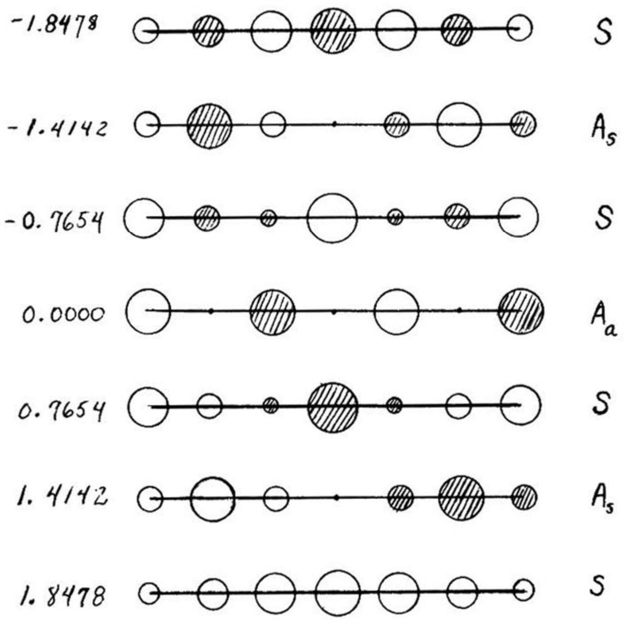

FIGURE 1. Eigenvalues and eigenvectors for the linear seven-vertex graph. Shaded circles refer to negative coefficients. Symbols at right indicate whether the eigenvector is symmetric (S) or antisymmetric (A) for reflection through the central vertex. The subscript refers to symmetry for reflection within each of the two subgraphs (i.e., within the three left-most or three right-most vertices.)

The perturbation operator for bridging c and a' by vertex v is $H' = \delta_{cv} + \delta_{a'v}$. This leads to mixing coefficients involving sums of products of the form $(c_i + a'_i)(c_j + a'_j)$. It follows immediately that any eigenvector having $c_i = -a'_i$ will not be affected by the perturbation and will not mix in with any eigenvectors that are affected. This means that the A_s eigenvectors in Fig. 1 are isolated from the perturbation and that their two corresponding eigenvalues will continue to be eigenvalues for the new graph 1.

We continue by considering the remaining five eigenvectors. Suppose ϕ_i and ϕ_j are both symmetric. Then $b_i=b'_i$, $b_j=b'_j$, and $b_i+\lambda b_j = b'_i+\lambda b'_j$, so the equivalence condition is met by mixing two symmetric eigenvectors. If ϕ_i or ϕ_j is antisymmetric (of the A_a type), then $b=b'=0$, so nothing happens to upset the equivalence condition.

It follows that we can guarantee equivalence preservation between sites if we have eigenvectors that meet all these symmetry conditions and if we bridge between the appropriate vertices. Note that bridging between a and c does not preserve b,b' equivalence. This results because now the A_s eigenvectors participate, and these eigenvectors have opposite signs at b and b', causing the equivalence condition to be lost. Note also that the A_a eigenvector fails to disrupt b,b' equivalence only because it has zero coefficients at b and b'. This happens only because b and b' are central atoms in an odd-numbered subchain.

II. Preservation of Equivalence between Two Pairs of Sites

Consider a five-vertex linear graph, 32, with eigenfunctions and eigenvalues indicated in Fig. 2. We have noted earlier that there are

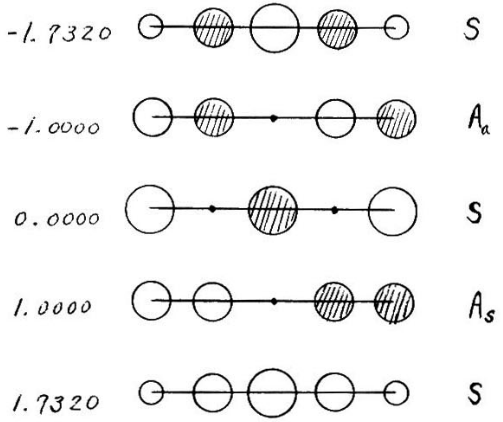

FIGURE 2. Eigenvalues, eigenvectors and symmetry symbols for the linear five-vertex graph. See Fig. 1 for definitions.

two ways to bridge this graph, a to b or a to b', and end up with a new graph having isospectral pairs of vertices (6 and 33 respectively). Before bridging, we have the following equivalent vertices: a with a', b with b', a+b with a'+b', a+b' with a'+b.

A. Bridging a to b'

Only the equivalence a+b with a'+b' survives. Therefore, we need to understand why the following equivalence condition is met in a to b' bridging:

$$|a_i + b_i + \sum_{j \neq i} \lambda_{j,i}(a_j + b_j)| = |a'_i + b'_i + \sum_{j \neq i} \lambda_{j,i}(a'_j + b'_j)|$$

As seen in part I, an A_s eigenvector is uninfluenced by the a–b' perturbation. (This requires symmetry in the subchains, such that |a|=|b|.) Its eigenvalue survives as one of the eigenvalues of 6.

The remaining eigenvectors can mix in various symmetry combinations. If ϕ_i and ϕ_j are both symmetric, then $a_i = a'_i$, $b_i=b'_i$, $a_j=a'_j$, $b_j=b'_j$, and the equivalence condition is met. If ϕ_i and ϕ_j are both A_a (only possible with a graph larger than 32), then $a_i=-a'_i=-b_i=b'_i$, ditto for j, and both sides of the equivalence condition vanish. (Even without the equality between $|a_i|$ and $|b_i|$, the equivalence condition would be met.) If ϕ_i is S and ϕ_j is A_a, then $a_i=a'_i$, $b_i=b'_i$, $a_j=-a'_j=-b_j=b_j$. Then $a_j+b_j=a'_j+b'_j=0$ and the equivalence condition is satisfied. (Without the equality between $|a_j|$ and $|b_j|$, the condition would not be satisfied.)

B. Bridging a to b

Only the equivalence a+b with a'+b' survives. The analysis is similar to part A, except now it is the A_a eigenvectors that cannot participate.

These analyses indicate that we can preserve pair equivalences if we choose starting graphs which can be symmetrically sliced by a plane into subgraphs (without bisecting edges) and if the pairs of vertices are symmetrically disposed within these subgraphs. Labeling these pairs a,b in one subgraph and a',b' in the other, bridging a-b keeps equivalent a+b' to a'+b. Bridging a-b' keeps equivalent a+b to a'+b'.

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