The Characteristic Polynomial as a Structure Discriminator

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We investigate use of the characteristic polynomial for discrimination of graphs. Here we consider acyclic graphs (trees) only, and in particular we consider trees without bridging vertices because no isospectral trees in which both graphs are without bridging vertices have been hitherto reported. However, we found the smallest such isospectral trees when $n = 15$. When the maximal valence is limited to four, so that graphs correspond to molecules of organic chemistry, the smallest isospectral (nonbridging) trees have $n =$ 19 vertices. The smallest pair of isospectral binary trees were found among trees having $n = 26$ vertices. By combining contraction of trees to proper trees (i.e., trees without bridging vertices) and subsequent pruning of proper trees one can in many cases determine if two trees are isomorphic or not from comparison of their characteristic polynomials.

INTRODUCTION

Characteristic polynomial, $\mathrm{Ch}(x) = (-1)^n \det(\mathbf{A} - \mathrm{I}\, x)$, where **A** is the adjacency matrix of a graph, has received considerable attention in the literature.[1,2] Collatz and Sinogowitz[3] were the first to report the failure of the characteristic polynomial to discriminate among graphs by pointing to several pairs of isospectral trees, the smallest shown in Figure 1. The lower part of Figure 1 illustrates the pruning procedure, the process in which all terminal edges are deleted.[4] Balasubramanian developed very efficient scheme for construction of the characteristic polynomial of trees using the pruning procedure.[5,6]

The occurrence of isospectral graphs is the rule rather than an exception. Schwenk[7] demonstrated that as n, which represents the number of vertices of a graph, increases to infinity the quotient of the number of isospectral trees to the number of all trees tends to 1, which justifies the title of his article "Almost all trees are isospectral". Construction of isospectral graphs was particularly facilitated by recognizing that a pair of isospectral graphs may have vertices which allow substitution of an arbitrary fragment without affecting the isospectral property for the pair of graphs.[8−10] Moreover there are single graphs (referred to as endospectral graphs) that have two (symmetry nonequivalent) vertices which allow substitution of arbitrary fragment which results in formation of isospectral graphs (trees).[11−13] It appears therefore that characteristic polynomial will be of little help as a structure discriminator.

Examination of isospectral trees reported in the literature reveals that all have vertices of degree $d = 2$, the so called bridging vertices. Hence, the presence of bridging vertices facilitates occurrence of isospectral graphs; at least this appears to be the case for trees. Among cyclic graphs one finds isospectral graphs which have no vertices of degree two as illustrated by the two isospectral cubic graphs reported

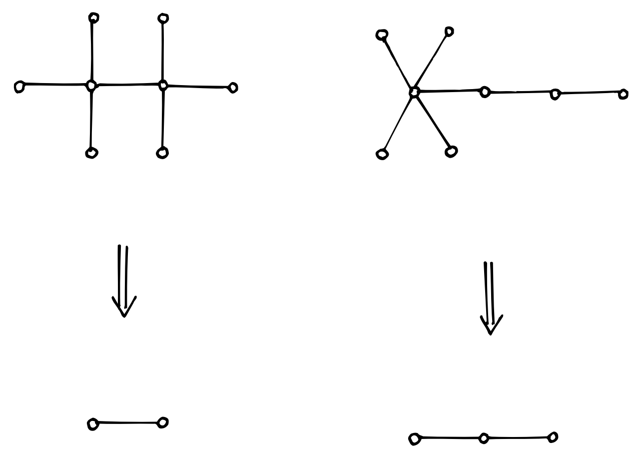

Figure 1. The smallest pair of isospectral trees.

by Schwenk.[14] However no isospectral trees without bridging vertices (the so called proper trees) were hitherto reported. Is it possible to have isospectral trees without the presence of ubiquitous bridging vertices? Are there isospectral binary trees or isospectral ternary trees, i.e., trees with the maximal valence $d = 3$ and $d = 4$, respectively? In this article we consider the above questions. The answer will help us to understand better the occurrence of isospectral graphs (trees). Moreover, it may help us in modifying use of the characteristic polynomial in facilitating in graph isomorphism testing, at least among the trees.

ISOSPECTRAL PROPER TREES

We have undertaken a systematic search for proper graphs that have identical characteristic polynomials. We have used the already outlined computer program that generates all trees and their characteristic polynomials which is based on n-tuple code for trees.[15,16] In Table 1 we show for trees having n vertices the number of characteristic polynomials appearing more than once. The trees are classified as (a) all trees; (b) alkanes (i.e., trees with the maximal valence four); (c) proper trees (i.e., trees with no vertices of degree two); (d) proper alkanes (i.e., trees with valence 1, 3, 4); and (e) binary trees

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Table 1. The Numbers Show Repeated Occurrence of the Same Characteristic Polynomial

n	all trees	alkanes	proper trees	proper alkanes	binary trees
7	0	0	0	0	0
8	1	0	0	0	0
9	5	5	0	0	0
10	4	2	0	0	0
11	29	21	0	0	0
12	56	43	0	0	0
13	192	124	0	0	0
14	390	254	0	0	0
15	1132	717	2	0	0
16	2405	1492	3	0	0
17	6628	3989	7	0	0
18	14615	8312	11	0	0
19	37458	20431	23	1	0
20	81779	43443	26	1	0
...	...	...	...	...	...
26	...	...	...	...	1

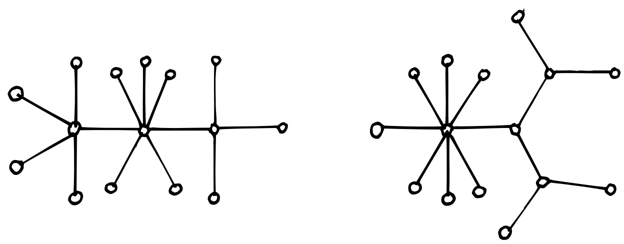

Figure 2. The smallest proper trees having the same characteristic polynomial.

(i.e., trees with all vertices of degree three except the terminal vertices of degree one).

Among the trees on $n = 15$ vertices we found the smallest isospectral proper trees (shown in Figure 2). The characteristic polynomial for the trees of Figure 2 is $x^{15} - 14x^{13} + 54x^{11} - 60x^9$, and the corresponding n-tuple codes are 740000300000000 and 822002000000000, respectively. The graphs of Figure 2 give the answer (negative) to the first question posed in the introduction.

If we restrict the maximal valence to $d = 4$ we find the smallest pair of isospectral trees representing alkanes to have $n = 19$ vertices (Figure 3). Their characteristic polynomial is $x^{19} - 18x^{17} + 123x^{15} - 403x^{13} + 664x^{11} - 488x^9 + 120x^7$. In Figure 4 (the upper part) is illustrated another pair of isospectral proper trees having $n = 20$ vertices. The characteristic polynomial of the pair of trees of Figure 4 is $x^{20} - 19x^{18} + 141x^{16} - 525x^{14} + 1040x^{12} - 1056x^{10} + 464x^8 - 48x^6$. As n increases the number of isospectral proper trees is likely to increase. It remains to see how the quotient of the number of isospectral proper trees to the total number of proper trees increases as n increases indefinitely. So far we have too few examples of isospectral proper trees to speculate about the presence of structural patterns underlying the isospecterality among such graphs.

Finally we made some computations and included as the last row of Table 1 the first pair of proper binary trees with the same characteristic polynomial. Their n-tuple codes are respectively 32222220020020022000020000 and 32222220020022002000200000. Their common characteristic polynomial is $x^{26} - 25x^{24} + 264x^{22} - 1540x^{20} + 5444x^{18} - 12020x^{16} + 16242x^{14} - 13200x^{12} + 5536x^{10} - 896x^8$. The two graphs are illustrated in Figure 5.

PRUNING OF PROPER TREES

Pruning of a tree is an operation in which terminal vertices (and incident terminal edges) are removed from a graph. In Figure 5 we illustrated the pruning for the pair of isospectral proper graphs having 20 vertices. Such a process will result typically in a tree with bridging vertices. A tree with bridging vertices can be condensed into a proper tree by a procedure in which vertices of degree two are ignored. This is illustrated in the lower part of Figure 4 for the pair of the pruned proper trees. By combing the two procedures one reduces a large proper tree to a smaller proper tree. If we start with a proper tree, pruning results in a smaller tree which may have bridging vertices, and if we start with a tree having bridging vertices by condensation, we end with smaller proper tree. In the case of a pair of isospectral trees the pruning followed by condensation will result in smaller proper trees that may be different or identical. As we see from Figure 5 in this particular case the pruning of two isospectral graphs resulted in an identical reduced proper tree.

We want to explore use of the characteristic polynomial for isomorphism testing of trees. Isomorphism testing is important for graphs because the same graphs can be represented in very many different pictorial forms or by many different matrices (the individual forms of which depend on the assumed numbering for vertices). There are many different schemes for checking graph isomorphism. For a review of earlier approaches to graph isomorphism problem see refs 17 and 18. A more recent method which uses the eigenvectors of the adjacency matrix has been outlined by Liu and Klein.[19]

If after a pair of isospectral trees are pruned and then condensed we obtain different proper trees, we may conclude that the initial graphs are not isomorphic. When the pruning and the condensation process applied to two isospectral trees result in the same proper graph, we may have nonisomorphic graphs or may have the same graph. It is possible to differentiate the two cases by keeping the record, i.e., the history of the pruning and the condensation. If the record is different for the two trees, they are nonisomorphic; if the history is identical, graphs represents a duplicate of the other. For the trees of Figure 5, however, the pruned trees are not isospectral, hence, the initial graphs are nonisomorphic.

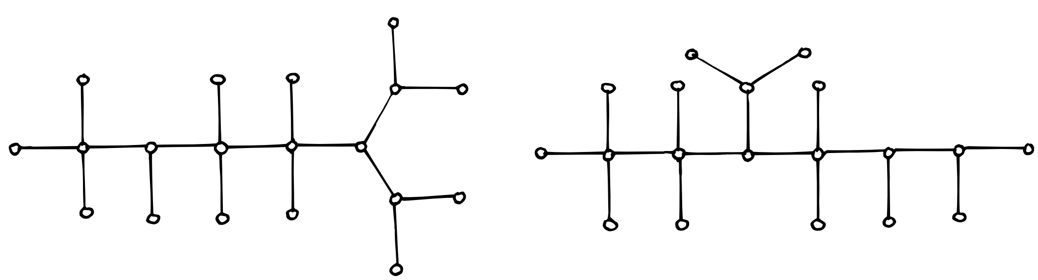

Figure 3. Isospectral proper trees with the maximal valence four ($n = 19$).

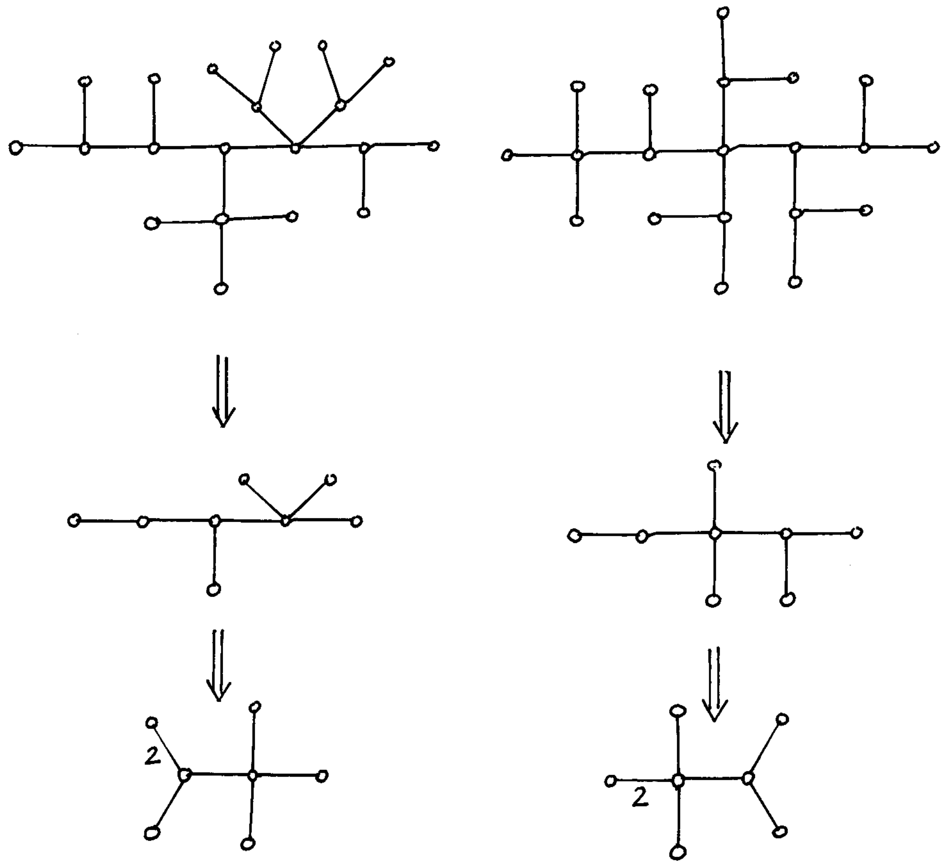

Figure 4. Pruning of isospectral proper trees with the maximal valence four ($n = 20$).

The record of the condensation process is kept by giving to the edges of the derived proper tree the weight depending on the number of the fused edges that the new edge represents. The record of the pruning process is kept by giving to the vertices of the derived pruned tree the weight depending on the number of the pruned edges that were deleted at the considered vertex. For two graphs of Figure 5 we see that the condensation results in giving the weight $w = 2$ to different terminal edges of the resulting proper tree—hence, the initial graphs are nonisomorphic.

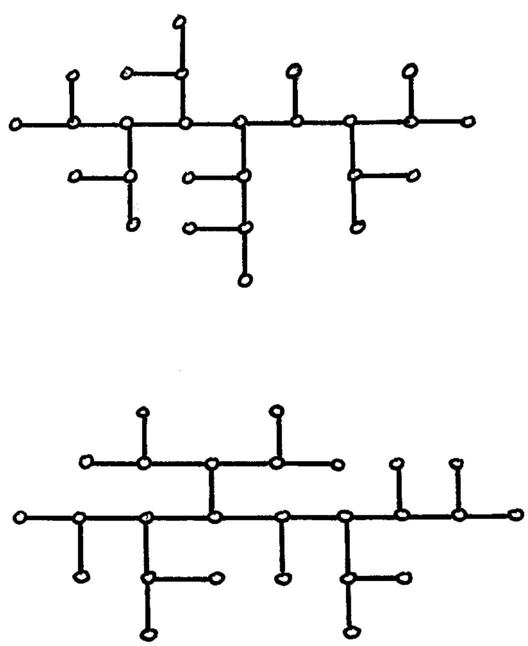

Figure 5. The smallest pair of isospectral binary trees ($n = 26$).

ILLUSTRATIONS

Many isospectral graphs are obtained from an endospectral tree by attaching the same fragment (for example, an edge) to either of the two endospectral points following the procedure initially outlined by Schwenk,[7] Herndon,[8] and Živković and collaborators.[9,10] If we want to test such a pair of graphs for isomorphism by condensation we could easily establish that they are distinct if the condensed proper graphs are different. If, however the resulting proper graphs are identical, further testing is required. Because of this situation it is of interest to investigate what structural factors cause some endospectral graphs to lead to the first case (an easy test) and what lead to the second case (that require more testing).

In Figure 6 we show all trivially unrelated endospectral graphs having from $n = 9$ to $n = 12$ vertices. They have been constructed or found by Schwenk,[7] Godsil, and McKay,[20] Knop and co-workers,[21] Randić and Kleiner,[12] Randić[22] and Jiang,[11] respectively. Here we excluded as trivial endospectral graphs that can be obtained from a smaller endospectral graph by introducing the same fragments to their respective endospectral points.

From the six endospectral graphs depicted in Figure 6 only the graph reported by Knop and collaborators[21] (reproduced in the traditional chemical form at the top of Figure 7) leads to a distinct reduced proper graph if used for construction of a pair of isospectral graph. As illustrated in Figure 7 we first constructed two isospectral trees by adding an edge at the positions 2 and 5 along the longest chain, respectively. When the two isospectral graphs are condensed to proper trees, they result in different proper trees (corresponding to

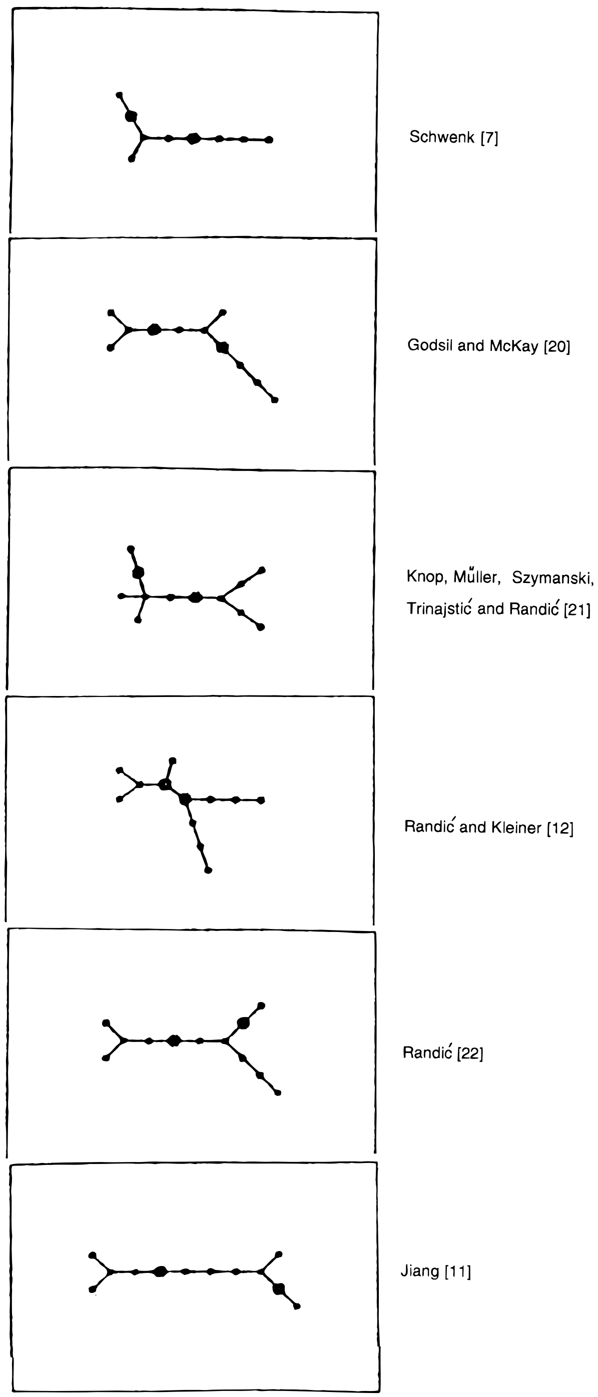

Figure 6. Endospectral graphs with $n = 9$ to $n = 12$ vertices.

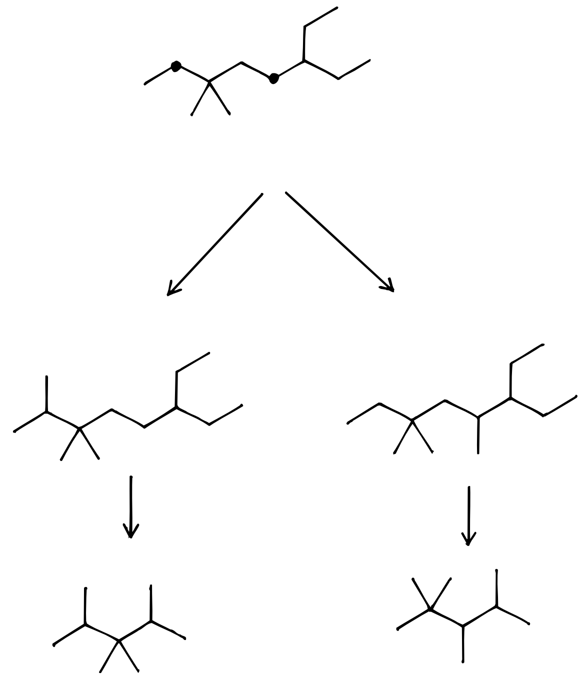

Figure 7. Reduction of isospectral trees to distinct proper trees.

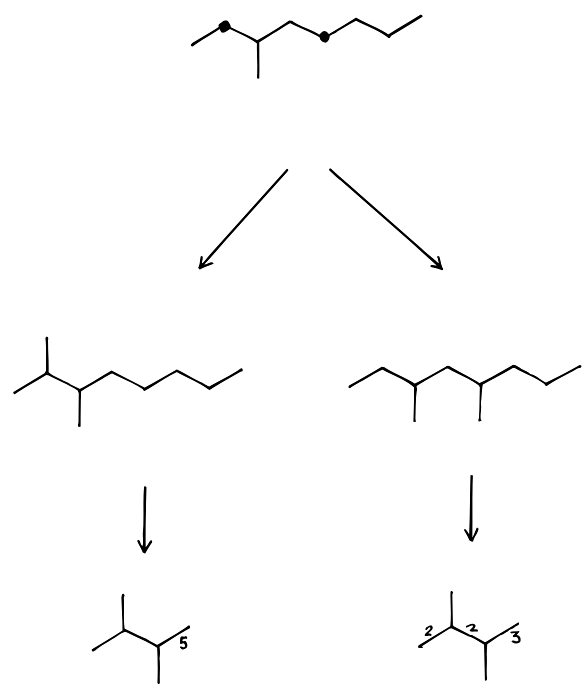

Figure 8. Reduction of isospectral trees to the same proper tree but having different edge weights.

2,3,3,4-tetramethylpentane and 2,2,3,4-tetramethylpentane). When the remaining five graphs of Figure 6 are used for construction of isospectral trees, the resulting isospectral trees are reduced to the same proper tree. In order to establish whether such graphs are isomorphic or not (assuming that we do not know how were they constructed), we have to assign to the reduced edges the corresponding weights determined by the number of condensed edges. If the weights are different, or the same but assigned to distinct symmetry nonequivalent edges, the graphs are nonisomorphic. This is illustrated (in Figure 8) for isospectral trees derived from Schwenk's endospectral tree. The following question may be raised: What causes such different behavior for different endospectral graphs.

CLASSIFICATION OF ENDOSPECTRAL TREES

In order to understand the structural factors involved in the differentiation between apparently similar endospectral trees we have examined larger endospectral trees (having from 13 to 16 vertices). All the endospectral trees considered were reported in ref 21. When these endospectral trees are used for construction of isospectral graphs in most cases, the pair of isospectral trees obtained by adding an edge to either of the two endospectral points reduces by condensation of the vertices of degree two to the same proper tree. The cases that do not reduce to the same tree have been collected in Figure 9. A closer look at Figure 9 suggests that the

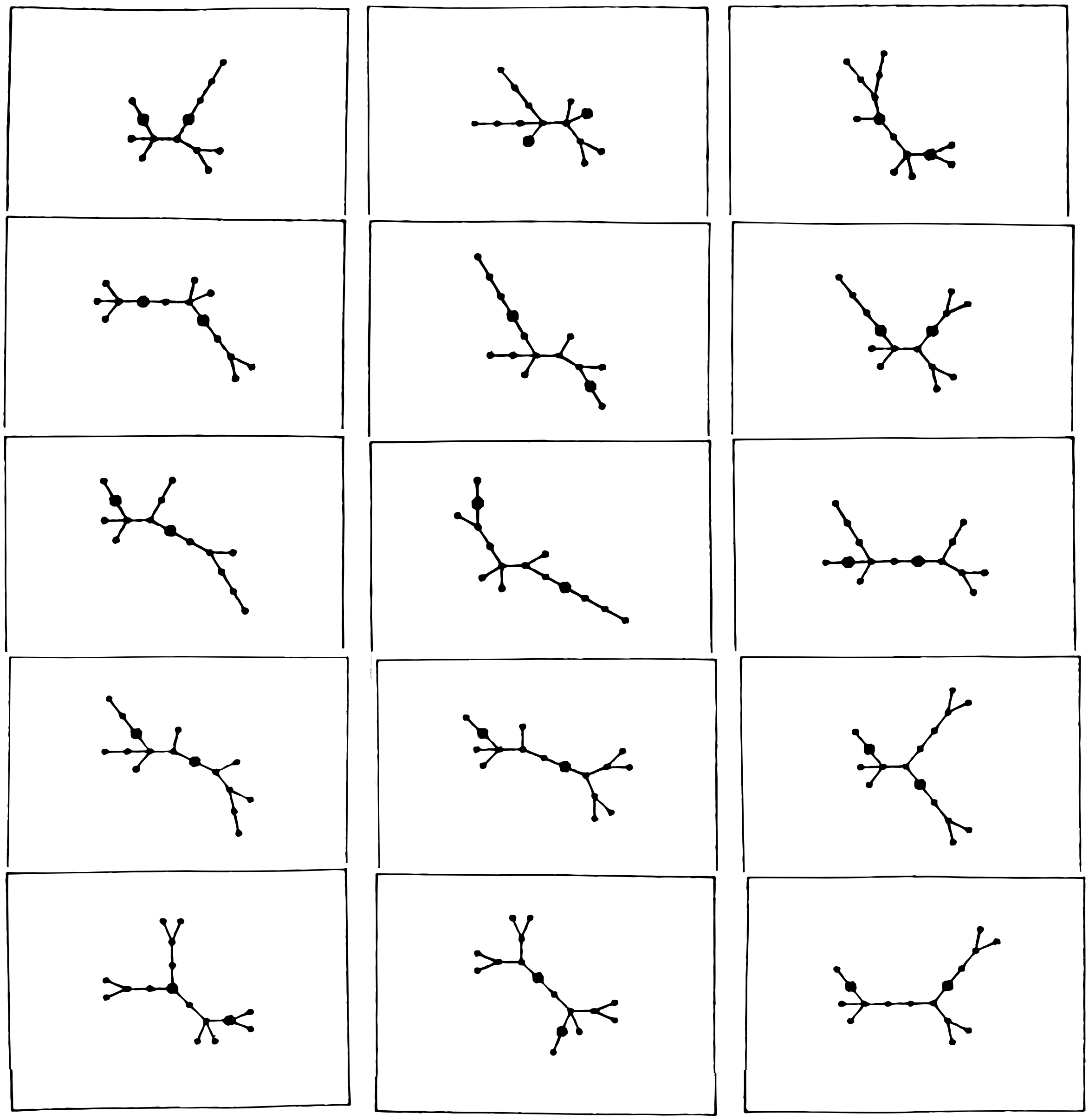

Figure 9. Endospectral trees having from $n = 13$ to $n = 16$ vertices.

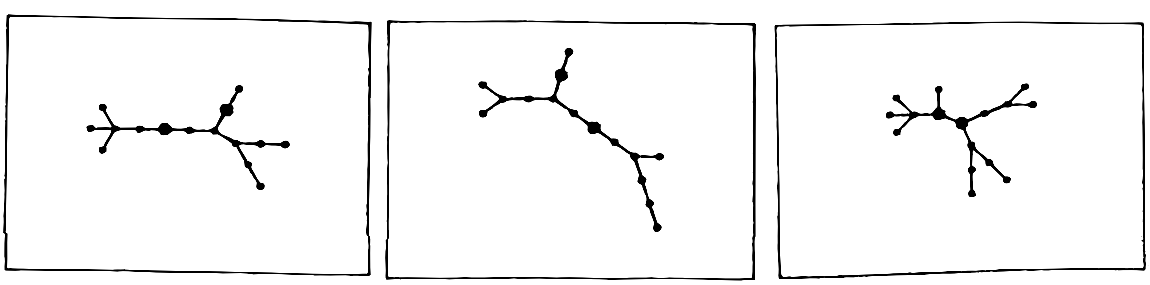

Figure 10. Endospectral trees with branched fragment between the endospectral points or with adjacent endospectral points.

presence of vertices of degree four between the two endospectral points may be the cause for the distinct behavior of such isospectral trees. All other endospectral trees (about 40) have no vertices of degree four *between* the two endospectral points. However, in addition to graphs of Figure 9 also the endospectral trees of Figure 10 (which do not have vertices of degree four between endospectral points) produce distinct reduced trees. In the case of graphs of Figure 10 the cause for the occurrence of different proper trees is the presence of branched fragment or the dissimilarity between the adjacent endospectral points. We can summarize our observations as follows:

Isospectral trees derived from a parent endospectral graph will reduce to the same proper graph if no vertices of degree four (or higher) occur between the endospectral points, if no branched fragments occur between the endospectral points, or if adjacent endospectral points have asymmetrically attached fragments. The above is true when isospectral graphs are obtained from the parent endospectral tree by substituting an edge or a path graph at the alternative endospectral points. If, however, instead of an edge or a path we insert a branch fragment at the isospectral point, the two isospectral trees will reduce in general to distinct proper trees.

ISOMORPHISM ALGORITHM

By combining the pruning and the condensation of trees and using the fact that there are no small ($N < 15$) isospectral proper trees and that there are no small proper alkanes ($N < 19$) and no proper small binary trees ($N < 26$) one can arrive at a useful procedure for testing trees for isomorphism:

(1) Find Ch(x) for two trees G_1 and G_2 considered. If different the graphs are nonisomorphic.

(2) If the two graphs have identical characteristic polynomials reduce the trees to proper trees. Test the reduced trees for Ch(x). If different, the graphs are nonisomorphic.

(3) If the two graphs have identical characteristic polynomials prune the trees. Test the pruned trees for Ch(x). If their characteristic polynomials are different, the graphs are nonisomorphic.

(4) If the two pruned graphs have identical characteristic polynomials continue the process of condensation and pruning till graphs are sufficiently small that by inspection one can see if the reduced graphs are identical or not. If the graphs are not identical, the original graphs are nonisomorphic. If graphs are identical, backtrack the pruning/condensation steps keeping the record of the condensation of the edges by giving them the weight according to the degree of condensation (as outlined in the previous section). If the weights derived from the two isospectral graphs are different, the graphs are nonisomorphic, otherwise the graphs are isomorphic.

The outlined procedure is not meant to replace the existing tests for isomorphism among trees but rather to supplement such. The advantage of the outlined procedure is that it can be used by most chemists without access to more sophisticated and elaborated isomorphism testing procedure. All that is required here is evaluation of the characteristic polynomial, which is readily available from most computer software (such as, e.g., MATLAB). Moreover, the characteristic polynomials of trees can also readily be evaluated without computers using graphical and graph theoretical methods[23,24] and using Chebyshev expressions for polynomials which allow relatively simple recursion forms of larger polynomials in terms of smaller ones in many cases.[25,26]

REFERENCES AND NOTES

(1) Randić, M.; Barysz, M.; Nowakowski, J.; Nikolić, S.; Trinajstić, N. Isospectral graphs revisited. *J. Mol. Struct. (Theochem)* **1989**, *185*, 95−121, and references therein.

(2) Cvetković, D. M.; Doob, M.; Sachs, H. Spectra of Graphs - Theory and Applications, 3rd revised and enlarged edition; Johann Ambrosius Barth Verlag: Heidelberg-Leipzig, 1995.

(3) Collatz, L.; Sinogowitz, U. Spektren endlichen Graphen. *Abh. Math. Sem.* University of Hamburg, **1957**, *21*, 63.

(4) Balasubramanian, K. Spectra of chemical trees. *Int. J. Quant. Chem.* **1982**, *21*, 581−590.

(5) Balasubramanian, K.; Randić, M. The characteristic polynomials of structures with pending bonds. *Theor. Chim. Acta* **1982**, *61*, 307−323.

(6) Balasubramanian, K. Tree pruning and lattice statistics on Bethe lattices. *J. Math. Chem.* **1988**, *2*, 69−82.

(7) Schwenk, A. J. Almost all trees are cospectral In *New Directions in the Theory of Graphs*; Harary, F., Ed.; Academic Press: New York, 1973; pp 275−307.

(8) Herndon, W. C. Isospectral molecules. *Tetrahedron Lett.* **1974**, 671−674.

(9) Živković, T.; Trinajstić, N.; Randić, M. On conjugated molecules with identical topological spectra. *Mol. Phys.* **1975**, *30*, 517−533.

(10) Randić, M.; Trinajstić, N.; Živković, T. On molecular graphs having identical spectra. *J. Chem. Soc. Faraday Trans. 2* **1976**, *72*, 244−256.

(11) Jiang, Y. Problems on isospectral molecules. *Sci. Sin. (Ser. B)* **1984**, *27*, 236.

(12) Randić, M.; Kleiner, A. F. On the construction of endospectral trees. *Ann. New York Acad. Sci.* **1989**, *555*, 320−331.

(13) Müller, W. R.; Szymanski, K.; Knop, J. V.; Mihalić, Z.; Trinajstić, N. Notes on isocodal graphs. *J. Chem. Inf. Comput. Sci.* **1995**, *35*, 871−873.

(14) Schwenk, A. J. Exactly thirteen connected cubic graphs have integral spectra. In *Theory and Applications of Graphs*; Proceedings of the Kalamazoo International Conference, Alavy Y., Lick D., Eds; Springer Verlag: Berlin-Heidelberg-New York, 1978.

(15) Knop, J. V.; Müller, W. R.; Jeričević, Z.; Trinajstić, N. Computer enumeration and generation of trees and rooted trees. *J. Chem. Inf. Comput. Sci.* **1981**, *21*, 91.

(16) Knop, J. V.; Müller, W. R.; Szymanski, K.; Trinajstić, N. Computer Generation of Certain Classes of Molecules. SKTH/Kemija u industriji: Zagreb, 1985.

(17) Read, R. C.; Corneil, D. G. The graph theory disease. *J. Graph Theory* **1977**, *1*, 339−363.

(18) Gati, G. Further annotated biography on the isomorphism disease. *J. Graph Theory* **1979**, *3*, 95−109.

(19) Liu, X.; Klein, D. J. The graph isomorphism problem. *J. Comput. Chem.* **1991**, *12*, 1243−1251.

(20) Godsil, C.; McKay, B. Some computational results on the spectra of graphs. *Lect. Notes Math.* **1976**, *560*, 72.

(21) Knop, J. V.; Müller, W. R.; Szymanski, K.; Trinajstić, N.; Kleiner, A. F.; Randić, M. On irreducible endospectral graphs. *J. Math. Phys.* **1986**, *27*, 2601−2612.

(22) Randić, M. Random walk and their diagnostic value for characterization of atomic environment. *J. Comput. Chem.* **1980**, *1*, 386−399.

(23) Hosoya, H. Graphical enumeration of the coefficients of the secular polynomials of the Huckel molecular orbitals. *Theor. Chim. Acta* **1972**, *25*, 215−222.

(24) Randić, M. On Evaluation of the characteristic polynomial for large molecules. *J. Comput. Chem.* **1982**, *3*, 421−435.

(25) Randić, M. On alternative form of the characteristic polynomial and the problem of graph recognition. *Theor. Chim. Acta* **1983**, *62*, 485−498.

(26) Hosoya, H.; Randić, M. Analysis of topological dependency of the characteristic polynomial in its Chebyshev expansion. *Theor. Chim. Acta* **1983**, *32*, 473−495.

(27) Randić, M.; Baker, B.; Kleiner, A. F. Factoring the characteristic polynomial. *Int. J. Quant. Chem.: Quant. Biol. Symp.* **1986**, *19*, 107−127.

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