THEORETICA CHIMICA ACTA
Theoret. Chim. Acta (Berl.) 62, 485–498 (1983)

Original Investigations

On Alternative Form of the Characteristic Polynomial and the Problem of Graph Recognition

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The characteristic polynomial of a structure (molecule or a graph) is usually expressed as a function of x. Here we explore an alternative representation of characteristic polynomials expressed in terms of L_n, the characteristic polynomials of linear chains having n atoms. While the new forms of the characteristic polynomials are mathematically equivalent to the old forms, they appear to reflect selected structural similarities among homologous molecules better. Besides arriving at general expressions for the form of the characteristic polynomials for numerous families of compounds previously unavailable, the approach is of some interest for the old problem of graph isomorphism and graph recognition in cases of structures which can be associated with a homologous series.

Key words: Characteristic polynomial-Graph isomorphism–Isospectral graphs – Graph recognition.

1. Introduction

The characteristic polynomial of a graph, defined as $(-)^n \det(A\text{-}xI)$, A being the adjacency matrix of a graph and I the unit matrix of the same dimension, is an important structural invariant. At one time it was expected that the characteristic polynomial characterizes the graph, that is, that two graphs are isomorphic if and only if the characteristic polynomials of their adjacency matrices are the same [1]. However, as Collatz and Sinogowitz had shown [2], in a paper only more recently widely cited, there are numerous instances of isospectral graphs, graphs which are nonisomorphic, yet have all eigenvalues identical, hence

* Operated for the U.S. Department of Energy by Iowa State University under contract no. W-7405-ENG-82. This work was supported in part by the Office of the Director.

identical characteristic polynomials. While this fact opened the topic of isospectral graphs [3], it considerably reduced interest in the characteristic polynomial as a descriptor of structures. The characteristic polynomials are still of much interest, not in the area of chemical documentation, rather as a source of information on a structure. The coefficients of the characteristic polynomial are related to count of random walks and self returning walks, count of non-adjacent numbers and even count of cycles [4]. König was first to relate elements of the expansion of a determinant to selected subgraphs and thus open the way to graph theoretical evaluations of a determinant [5]. In 1950 Coulson illustrated how the coefficients of the secular determinant (for a Hückel MO-type calculations) can be evaluated by counting selected subgraphs of a molecular graph [6]. Pictorial expansion of the characteristic polynomial was later outlined by Spialter [7] and a systematic approach was offered by Sachs [8]. The general expression for the coefficients of the characteristic polynomial is elegant: they are given as a combination of subgraphs constructed from disjoint lines or cycles. However, already in case of structures having a dozen atoms the number of combinatorial possibilities that ought to be counted is too large, and application of the theorem becomes impractical. More recently a number of simplifying modifications have been suggested, such as contraction of a graph by suitable weighting factors assigned to bonds and vertices [9], use of a composition principle [10], and pruning of terminal bonds [11] or terminal fragments [12] and thus reducing the size of graphs dramatically. Finally, it was proposed to seek fewer but larger fragments as components for the construction of the characteristic polynomial [13]. This offsets the explosive increase in the number of combinations to be considered when individual bonds and cycles are used as components instead. In order to keep the number of distinctive components small, the characteristic polynomials of trees (i.e., acyclic graphs) were all expressed in terms of the characteristic polynomials of linear chains of different length. In one of his earlier work on Hückel MO Heilbronner [14] considered linear chains and derived recurrent expression for the chains and for the cycles, in terms of the chains, but these served only as auxiliary expressions, the tabulated characteristic polynomials were all expressed in terms of x^i powers. Here we will explore use of $L_n(x)$ polynomials, which are the characteristic polynomials for chains of length n and express characteristic polynomials of other structures in terms of L_n. In particular we will (1) consider larger acyclic structures; (2) consider numerous cyclic structures with pending bonds; and (3) extend the application to families of structurally related graphs. Mathematically the two forms of the characteristic polynomial, one expressed in powers of x and the other expressed in terms of L_n polynomials, are equivalent. As will be seen, the latter forms, on comparison of structurally related systems, show more visibly the similarities and therefore open a route to general expression for the characteristic polynomial for a family of structurally related molecules. Explicit forms for $L_n(x)$ have already been reported by Collatz and Sinogowitz:

$$L_n(x) = \sum_{m=0}^{[n/2]} (-1)^m \binom{n-m}{m} x^{n-2m}$$

and can be found tabulated for $n = 1,20$ in a review article by Trinajstić [15] on construction of characteristic polynomials. $L_n(x)$ are in fact Chebyshev polynomials in $x/2$, usually labeled as $T_n(x/2)$.

2. Acyclic Structures

Since the characteristic polynomials for acyclic graphs are known [16] one can derive the equivalent forms expressed in terms of L_n by first expressing various powers of x in terms of L_n and then make a straightforward substitution. For

Table 1. Characteristic polynomials of C_9 isomers expressed as a linear combination of polynomials L_n

Isomer	Characteristic polynomial
n-nonane	L_9
2-methyloctane	L_9-L_5
3-methyloctane	$L_9-L_5-L_3$
4-methyloctane	$L_9-L_5-L_3-L_1$
3-ethylheptane	$L_9-L_5-2L_3-L_1$
4-ethylheptane	$L_9-L_5-2L_3-2L_1$
2,6-dimethylheptane	$L_9-2L_5+L_1$
2,5-dimethylheptane	$L_9-2L_5-L_3+L_1$
2,4-dimethylheptane	$L_9-2L_5-L_3-L_1$
3,5-dimethylheptane	$L_9-2L_5-2L_3$
2,3-dimethylheptane	$L_9-2L_5-2L_3-L_1$
2-methyl-4-ethylhexane	same
3,4-dimethylheptane	$L_9-2L_5-3L_3-2L_1$
2-methyl-3-ethylhexane	$L_9-2L_5-3L_3-3L_1$
3-methyl-4-ethylhexane	$L_9-2L_5-4L_3-3L_1$
2,2-dymethylheptane	$L_9-3L_5-2L_3$
2,3,5-trimethylhexane	same
3,3-trimethylheptane	$L_9-3L_5-4L_3-2L_1$
2,3,4-trimethylhexane	same
4,4-dimethylheptane	$L_9-3L_5-4L_3-4L_1$
2,4-dimethyl-3-ethylhexane	same
3-methyl-3-ethylhexane	$L_9-3L_5-6L_3-5L_1$
3,3-diethylpentane	$L_9-3L_5-8L_3-7L_1$
2,2,5-trimethylhexane	$L_9-4L_5-2L_3+3L_1$
2,2,4-trimethylhexane	$L_9-4L_5-3L_3+L_1$
2,4,4-trimethylhexane	$L_9-4L_5-4L_3-L_1$
2,2,3-trimethylhexane	$L_9-4L_5-5L_3-3L_1$
2,3,3-trimethylhexane	$L_9-4L_5-6L_3-5L_1$
2,2-dimethyl-3-ethylpentane	same
3,3,4-trimethylhexane	$L_9-4L_5-7L_3-5L_1$
2,3-dimethyl-3-ethylpentane	$L_9-4L_5-8L_3-7L_1$
2,2,3,4-tetramethylpentane	$L_9-5L_5-6L_3-2L_1$
2,3,3,4-tetramethylpentane	$L_9-5L_5-8L_3-6L_1$
2,2,4,4-tetramethylpentane	$L_9-6L_5-4L_3+5L_1$
2,2,3,3-tetramethylpentane	$L_9-6L_5-10L_3-7L_1$

example from:

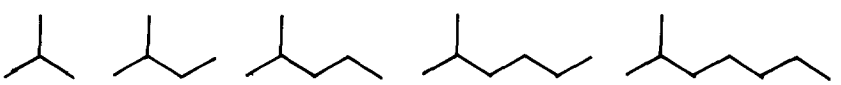
$$L_1 = x$$
$$L_2 = x^2 - 1$$
$$L_3 = x^3 - 2x \text{ etc.},$$

one immediately obtains:

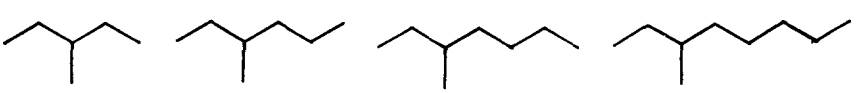
$$x = L_1$$
$$x^2 = L_2 + 1$$
$$x^3 = L_3 + 2L_1 \text{ and so on.}$$

In Table 1 we give the characteristic polynomials for isomers of nonane C_9H_{20}. Some regularities can be seen already by inspection of the Table 1. The coefficient of L_5 is reflecting the number and type of substitution of the main chain: -1 for methyl group; -2 for dimethyl substitution at two different carbon atoms or similar methyl-ethyl substitution; -3 for dimethyl substitution on a same carbon atom and methyl-ethyl substitution on a same carbon atom; -4 for disubstituted carbon atoms and another substituted carbon atom; -5 for tetramethyl substituted pentane one carbon atom having double substitution, and finally -6 for tetramethyl substituted pentane with two atoms having double substitution. It is more difficult to discern regularities in other coefficients, primarily because the skeletal forms for isomers are so diverse. It seems therefore better to consider families of structurally related skeletal forms. In Table 2 we have collected

Table 2. Characteristic polynomials for selected families of branched alkanes expressed as function of L_n and as function of x^n

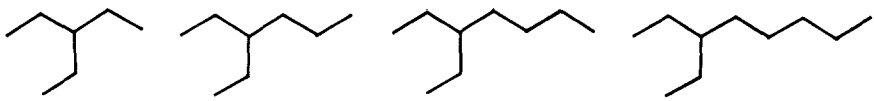


$L_4 - 1$	$x^4 - 3x^2$
$L_5 - L_1$	$x^5 - 4x^3 + 2x$
$L_6 - L_2$	$x^6 - 5x^4 + 5x^2$
$L_7 - L_3$	$x^7 - 6x^5 + 9x^3 - 2x$
$L_8 - L_4$	$x^8 - 7x^6 + 14x^4 - 7x^2$
$L_9 - L_5$	$x^9 - 8x^7 + 20x^5 - 16x^3 + 2x$
$L_{10} - L_6$	$x^{10} - 9x^8 + 27x^6 - 30x^4 + 9x^2$
$L_{11} - L_7$	$x^{11} - 10x^9 + 35x^7 - 50x^5 + 25x^3 - 2x$
$L_{12} - L_8$	$x^{12} - 11x^{10} + 44x^8 - 77x^6 + 55x^4 - 11x^2$

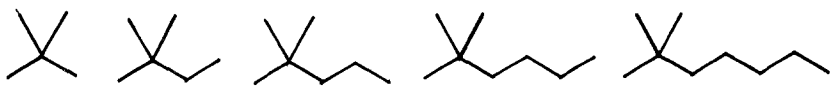


$L_6 - L_2 - 1$	$x^6 - 5x^4 + 5x^2 - 1$
$L_7 - L_3 - L_1$	$x^7 - 6x^5 + 9x^3 - 3x$
$L_8 - L_4 - L_2$	$x^8 - 7x^6 + 14x^4 - 8x^2 + 1$
$L_9 - L_5 - L_3$	$x^9 - 8x^7 + 20x^5 - 17x^3 + 4x$
$L_{10} - L_6 - L_4$	$x^{10} - 9x^8 + 27x^6 - 31x^4 + 12x^2 - 1$
$L_{11} - L_7 - L_5$	$x^{11} - 10x^9 + 35x^7 - 51x^5 + 29x^3 - 5x$
$L_{12} - L_8 - L_6$	$x^{12} - 11x^{10} + 44x^8 - 78x^6 + 60x^4 - 17x^2 + 1$

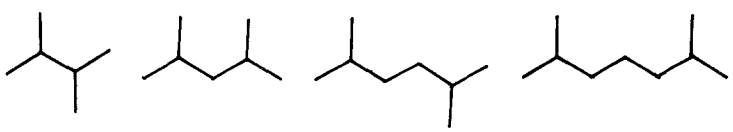
Table 2—*continued*



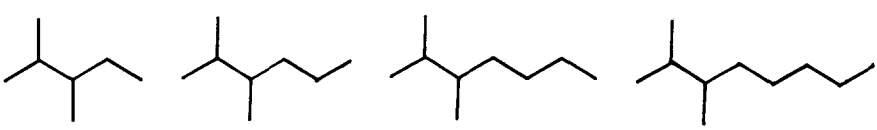
$L_7-L_3-2L_1$	$x^7-6x^5+9x^3-4x$
$L_8-L_4-2L_2-1$	$x^8-7x^6+14x^4-9x^2+1$
$L_9-L_5-2L_3-L_1$	$x^9-8x^7+20x^5-18x^3+5x$
$L_{10}-L_6-2L_4-L_2$	$x^{10}-9x^8+27x^6-32x^4+14x^2-1$
$L_{11}-L_7-2L_5-L_3$	$x^{11}-10x^9+35x^7-52x^5+32x^3-6x$
$L_{12}-L_8-2L_6-L_4$	$x^{12}-11x^{10}+44x^8-78x^6+60x^4-17x^2+1$



L_5-3L_1	x^5-4x^3
L_6-3L_2-2	$x^6-5x^4+3x^2$
$L_7-3L_3-2L_1$	$x^7-6x^5+7x^3$
$L_8-3L_4-2L_2$	$x^8-7x^6+12x^4-3x^2$
$L_9-3L_5-2L_3$	$x^9-8x^8+25x^6-22x^4+3x^2$
$L_{10}-3L_6-2L_4$	$x^{10}-9x^8+25x^6-22x^4+3x^2$
$L_{11}-3L_7-2L_5$	$x^{11}-10x^9+33x^7-40x^5+13x^3$
$L_{12}-3L_8-2L_6$	$x^{12}-11x^{10}+42x^8-65x^6+35x^4-3x^2$



L_6-2L_2-1	$x^6-5x^4+4x^2$
L_7-2L_3	$x^7-6x^5+8x^3$
L_8-2L_4+1	$x^8-7x^6+13x^4-4x^2$
$L_9-2L_5+L_1$	$x^9-8x^7+19x^5-12x^3$
$L_{10}-2L_6+L_2$	$x^{10}-9x^8+26x^6-25x^4+4x^2$
$L_{11}-2L_7+L_3$	$x^{11}-10x^9+34x^7+44x^5-16x^3$
$L_{12}-2L_8+L_4$	$x^{12}-11x^{10}+43x^8-70x^6+41x^4-4x^2$



$L_7-2L_3-2L_1$	$x^7-6x^5+8x^3-2x$
$L_8-2L_4-2L_2-1$	$x^8-7x^6+13x^4-6x^2$
$L_9-2L_5-2L_3-L_1$	$x^9-8x^7+19x^5-14x^3+2x$
$L_{10}-2L_6-2L_4-L_2$	$x^{10}-9x^8+26x^6-27x^4+8x^2$
$L_{11}-2L_7-2L_5-L_3$	$x^{11}-10x^9+34x^7-46x^5+22x^3-2x$
$L_{12}-2L_8-2L_6-L_4$	$x^{12}-11x^{10}+43x^8-72x^6+49x^4-10x^2$

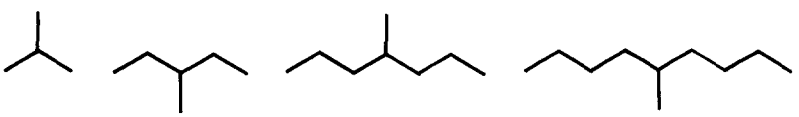
characteristic polynomials expressed in terms of x^i and L_n for a number of families of simply related structures. The first is the family of 2-methyl substituted alkanes. Although in this case the forms of the characteristic polynomial show a regularity, the equivalent expressions in terms of L_n are more simpler. With

Table 3. General expressions for the characteristic polynomials for branched alkanes of Table 2. The last column shows the smallest size of graph for which the expression holds

Substitution	General expression	n_{min}
2-methyl	$L_n - L_{n-4}$	4
3-methyl	$L_n - L_{n-4} - L_{n-6}$	6
3-ethyl	$L_n - L_{n-4} - 2L_{n-6} - L_{n-8}$	8
2,2-dimethyl	$L_n - 3L_{n-4} - 2L_{n-6}$	6
2,$(n-1)$-dimethyl	$L_n - 2L_{n-4} + L_{n-8}$	8
2,3-dimethyl	$L_n - 2L_{n-4} - 2L_{n-6} - L_{n-8}$	8

two substitutents and even with a single substitutent but at position 3 the characteristic polynomials become more involved and it takes more members of the family in order to discern the patterns for the coefficients. Nevertheless, when the characteristic polynomials are expressed in terms of L_n the resulting expressions are much simpler and allow one to write general expression already

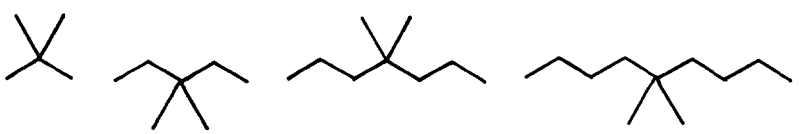
Table 4. Families of structures in which branching occurs at the center and their characteristic polynomials. Linear and nonlinear expression for the characteristic polynomial in terms of L_n are shown



$L_4 - 1$
$L_6 - L_2 - 1$
$L_8 - L_4 - L_2 - 1$
$L_{10} - L_6 - L_4 - L_2 - 1$

or

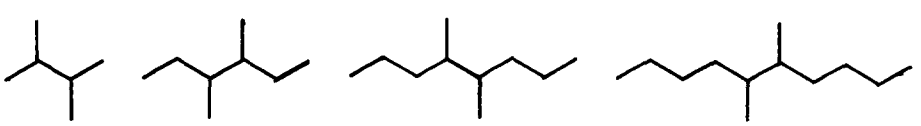
$L_1L_3 - (L_1)^2$
$L_1L_5 - (L_2)^2$
$L_1L_7 - (L_3)^2$
$L_1L_9 - (L_4)^2$



$L_5 - 3L_1$
$L_7 - 3L_3 - 4L_1$
$L_9 - 3L_5 - 4L_3 - 4L_1$
$L_{11} - 3L_7 - 4L_5 - 4L_3 - 4L_1$

or

$L_1(L_1L_3 - 2(L_1)^2)$
$L_1(L_1L_5 - 2(L_2)^2)$
$L_1(L_1L_7 - 2(L_3)^2)$
$L_1(L_1L_9 - 2(L_4)^2)$

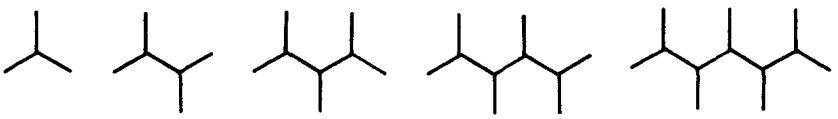


$L_6 - 2L_2 - 1$
$L_8 - 2L_4 - 3L_2 - 1$
$L_{10} - 2L_6 - 3L_4 - 3L_2 - 1$
$L_{12} - 2L_8 - 3L_6 - 3L_4 - 3L_2 - 1$

or

$(L_1)^2L_4 - L_1L_2(L_1 - 1)$
$(L_1)^2L_6 - L_2L_3(L_1 - 1)$
$(L_1)^2L_8 - L_3L_4(L_1 - 1)$
$(L_1)^2L_{10} - L_4L_5(L_1 - 1)$

Table 5. A family of structures with branching at every vertex (except terminal)



L_4-1	x^4-3x^2
L_6-2L_2-1	$x^6-5x^4+4x^2$
$L_8-3L_4-3L_2-1$	$x^8-7x^6+12x^4-4x^2$
$L_{10}-4L_6-5L_4-2L_2$	$x^{10}-9x^8+24x^6-20x^4+4x^2$

after deriving first few members. In Table 3 we have summarized the recurrent relations for the families of compounds considered in Table 2.

For the compounds of Table 2 the substitution sites are near one of the ends of the main chain, thus as the size of the graph increases more and more prominent is the "chain" as the dominant part of the structure. It is therefore not suprising to find that Chebishev polynomials in form of $L_n(x)$ play important role. If the site of the substitution is not at ends of the chains, but rather somewhere in the middle, one can nevertheless in number of cases recognize the pattern in the expressions for the characteristic polynomials and derive a general expression. As illustrated in Table 4 with selected families of compounds the expressions for the characteristic polynomials in the form of L_n components has now a somewhat more complex appearance. We have, in addition to the forms which are linear in L_n, also shown alternative expressions based on nonlinear terms which better portray the regularities within such families. Non-linear terms can be transformed into linear ones by repeated use of pertinent recurrent relations.

Finally, if one consider a family of compounds, such as one shown in Table 5, in which all sites are substituted, not suprisingly, the form of the characteristic polynomial as a function of L_n is becoming more involved and many members of the family need to be considered before one can discern correct pattern in the coefficients of various L_n terms.

3. Cyclic Structures

The same approach can be applied to cyclic and polycyclic structures. In Table 6 we have listed the characteristic polynomials expressed in terms of L_n for all monocyclic compounds having $n = 6$ and less vertices. Similarly in Table 7 and Table 8 results for families of structures are given: members differ by the length of the exocyclic chain and members differ by the size of the ring respectively. With a cycle a compound can correspond to bipartite or nonbipartite type and this is reflected in the parity of the components L_n. For bipartite graphs all terms have either even or odd subscript, depending on the number of vertices. It is of interest to compare the new forms for the characteristic polynomials as function of L_n and old forms as function of x^n. In Table 7 comparison is made for

Table 6. Monocyclic structures having six or less atoms and their characteristic polynomials as function of L_n

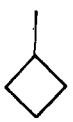
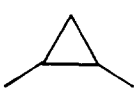
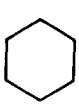
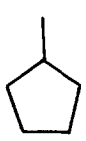
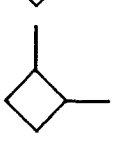
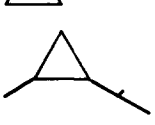
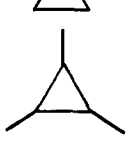
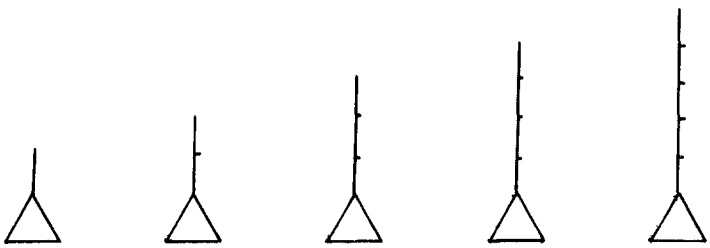
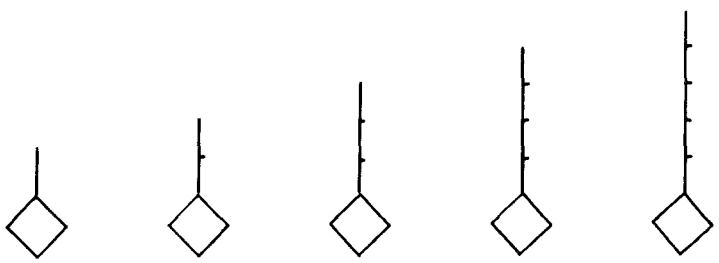
$n=3$			
	x^3-3x-2 L_3-L_1-2		
$n=4$			
	x^4-4x^2 L_4-L_2-2		x^4-4x^2-2x+1 $L_4-L_2+2L_1-1$
$n=5$			
	x^5-5x^3+5x-2 L_5-L_3-2		x^5-5x^3+2x $L_5-L_3-3L_1$
	$x^5-5x^3-2x^2+4x+2$ $L_5-L_3+2L_2-L_1$		$x^5-5x^3-2x^2+2x$ $L_5-L_3-2L_2-3L_1-2$
	$x^5-5x^3-2x^2+3x$ $L_5-L_3+2L_2-2L_1+2$		
	L_6-L_4-2		$L_6-L_4-L_2+2L_1$
	$L_6-L_4-3L_2-1$		$L_6-L_4-4L_2-2$
	$L_6-L_4-4L_2-3$		$L_6-L_4-5L_2-3$
	$L_6-L_5+2L_3-L_2$		$L_6-L_5+2L_3-2L_2$
	$L_6-L_4+2L_3-2L_2+2L_1-1$		$L_6-L_4+2L_3-3L_2+4L_1-2$
	$L_6-L_4+2L_3-3L_2+2L_1-2$		$L_6-L_4+2L_3-4L_2+4L_1-2$

Table 7. Characteristic polynomials for selected cyclic structures with pending linear chains (Initial members characteristic polynomials expressed as function of x^n can be found in: K. Kawasaki, K. Mizutani and H. Hosoya, Nat. Sci. Report Ochanomizu University **22**, 181 (1971), the higher polynomials were derived using recently outlined algorithm [20])



$L_4-L_2-2L_1-1$	x^4-4x^2-2x+1
$L_5-L_3-2L_2-L_1$	$x^5-5x^3-2x^2+4x+2$
$L_6-L_4-2L_3-L_2$	$x^6-6x^4-2x^3+8x^2+4x-1$
$L_7-L_5-2L_4-L_3$	$x^7-7x^5-2x^4+13x^3+6x^2-5x+2$



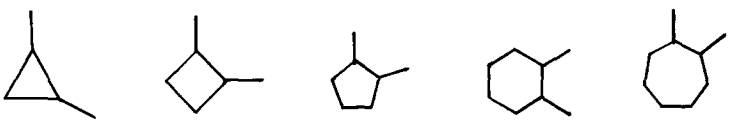
$L_5-L_3-3L_1$	x^5-5x^3+2x
$L_6-L_4-3L_2-1$	$x^6-6x^4+6x^2$
$L_7-L_5-3L_3-L_1$	$x^7-7x^5+11x^3-2x$
$L_8-L_6-3L_4-L_2$	$x^8-8x^6+17x^4-8x^2$

structures with a chain attached to a ring. The simplicity of expressions based on L_n is here very pronounced. One can immediately write down the next line, the characteristic polynomial for the next member in the family as function of L_n. To figure out correctly the coefficients of the characteristic polynomials for successive members of both families shown in Table 7 is not trivial and requires information on several additional members of the family in order to make sure that the suspected pattern is correct one.

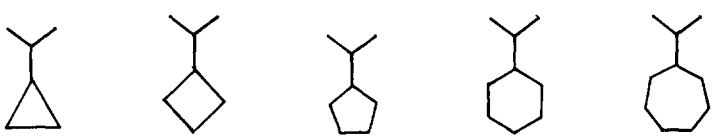
The results in Table 8 illustrate the effects of gradual increase of the ring size. Observe that in the considered cases there is a constant contribution of $2L_2+2$ or $-2L_2-2$ and a variable part which changes with change of the ring size. In summary, we see that the simplifications introduced with L_n as terms for expressing the characteristic polynomials of acyclic structures also extends to cyclic structures. Hence, although mathematically equivalent the new forms deserve more attention because they allow a more direct interpretation of algebra and topology of a structure.

Table 8. Examples of families of structures with rings of increasing size and their characteristic polynomials

$L_5-L_3-3L_1-2L_2-2$
$L_6-L_4-3L_2-1-2L_2-2$
$L_7-L_5-3L_3-L_1-2L_2-2$
$L_8-L_6-3L_4-L_2-2L_2-2$
$L_9-L_7-3L_5+L_3-2L_2-2$



$L_5-L_3-2L_1-2L_2-2$
$L_6-L_4-2L_2-1-2L_2-2$
$L_7-L_5-2L_3-L_1-2L_2-2$
$L_8-L_6-2L_4-L_2-2L_2-2$
$L_9-L_7-2L_5-L_3-2L_2-2$



$L_6-L_4-2L_2-2L_3$
$L_7-L_5-2L_3-L_1-2L_3$
$L_8-L_6-2L_4-L_2-1-2L_3$
$L_9-L_7-2L_5-L_3-L_1-2L_3$
$L_{10}-L_8-2L_6-L_4-L_2-2L_3$
$L_{11}-L_9-2L_7-L_5-L_3-2L_3$
$L_{12}-L_{10}-2L_8-L_6-L_4-2L_3$

4. On the Problem of Recognition

The problem of graph recognition – which we *here* distinguish from the problem of graph isomorphism – we define as the problem of identifying a given *single* structure as a structure previously recorded or assumed known. Consider for example the diagrams in Fig. 1. It is not difficult to recognize the top row as graphs representing a cube, but the last two diagrams (the bottom row) require some analysis and verifications before they are recognized as graphs representing the connectivity of a cube. By assuming a graph as "familiar" we understand that several of its properties are known to us, and when an "unknown" graph shows same properties we may suspect isomorphism, test it for isomorphism, and if confirmed, claim the graph being "recognized". Graph isomorphism is concerned with establishing whether or not two given graphs have identical connectivity. It is known that the graph isomorphism problem is difficult [19]

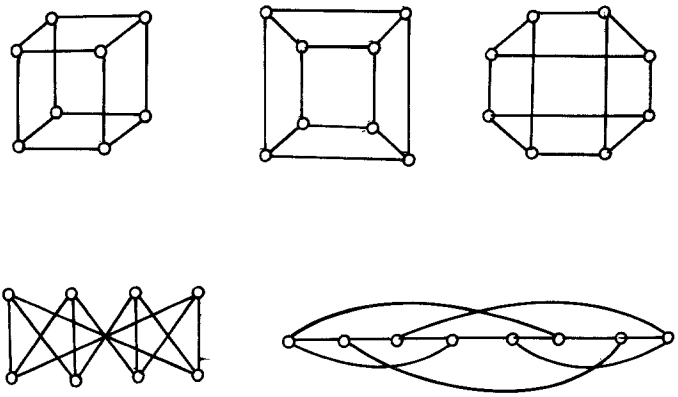


Fig. 1. Alternative forms for graph depicting the connectivity of a cube

and is still the subject of considerable interest [20]. The graph recognition problem as defined here may appear straightforward task – all one has to do is screen the files until coincidence occurs. This assumes some unique names have been deviced for structures, but difficulties are known when size of structures increases and when one allows even more general graphs, graphs not necessarily representing molecular skeletons to be considered. Even if one succeed in prescribing unique labels and names for graphs, such as based on canonical numbering of vertices [21], searching large files may not be the most efficient way of retrieval of "known" information. Most significantly one sometimes "recognizes" a novel structure, not previously considered at all, on the basis of its relation to some simpler structures. For example the first time that graph of a four-dimensional cube has been recognized as such was clearly accomplished by "analogy" with ordinary cube and its properties in three-dimensional space. Hence, the process of recognition has besides searching a memory also a heuristic component. Many structures and objects are recognized because related simpler structures have appeared elsewhere previoulsy. In the case of the four dimensional cube we observe that the number of vertices has doubled and that the structure can be viewed as two interconnected cubes. So, for recognition of graphs, it appears that *local* properties are of interest. Graph spectra reflects some local structural features, if nodal properties of graphs are closely examined [22]. Since spectra and characteristic polynomial are intimately connected one anticipates that characteristic polynomial, although global, may reflect some local structural features and thus offer a tool for graph recognition as here defined. Let's illustrate the spirit of the approach. The question to consider is as follows: given the characteristic polynomail, what can be said about the associated structure [23]? Clearly one cannot in general reconstruct the graph from the polynomial, since the latter is not unique. However we contend that some partial information can be extracted and in some cases even the structure can be recovered. For example consider 2-methyl substituted alkanes, the characteristic polynomial of which has the form $Ch(G_n) = L_n - L_{n-4}$. If one compares the structures and polynomials one sees that $(n-4)$ indicates the length of the

terminal chain, by defining the "end" group as having the four atoms as in the first structure of the family (isopropane). Similarly, in the case of 3-methyl substituted alkanes, the general expression $Ch(G_n) = L_n - L_{n-4} - L_{n-6}$, the length of the chain in successive members of the family, is given by $n-6$. Quite generally, if one comes across a polynomial the last term of which is not constant, one can relate the structure to a simpler one with k bridging vertices if the end term was L_k. The vertices need not be part of the end chain, but could, as in the case of alkanes with substituents on both ends, be inserted in between. One practical benefit of such considerations is that if one is constructing a file of structures of interest, one need only include a few initial members of a family. These would suffice for all members by use of the general term as a key for recognition. In using the characteristic polynomial for graph recognition, one has to be constantly aware that occurance of isospectral graphs may result in detecting only one such structure. For instance the polynomials $L_n - 3L_{n-4} - 2L_{n-6}$ belong to 2,2-dimethyl substituted alkanes, and when $n=9$ is specified, it will locate 2,2-dimethylheptane, but the characteristic polynomial $L_9 - 3L_5 - 2L_3$ also belongs to its isospectral pair: 2,3,5-trimethylhexane. The latter, however *is not* the member of this family. Equally, one can consider 2,3,5-trimethylhexane as a member of another family. One can select 2,3,5-trisubstituted alkanes or alternatively consider 2,3 substitutions and third substituent at $n-1$ position. The general terms for these families will produce 2,3,5-trimethylhexane without indicating that the graph may have an isospectral partner. Clearly, isospectral graphs appear as the intersection of two families.

Hence, it appears that if one can associate a structure with a family of compounds one might have unique characterization of the structure by its characteristic polynomial, if the polynomial is derived from a general expression for all members of the family. This raises hopes that the characteristic polynomial, which can be replaced by more readily available eigenvalues, can offer the basis and assist one in resolving even the problem of graph isomorphism, not alone, of course, but combined with the information for series of homologous compounds, of which the structure in question is member. Application of such an approach raises several interesting questions. Can two graphs with terminal chains (i.e., having at least chains with two vertices) and which are isospectral, produce isospectral pairs by reduction of the chain length? The number of known isospectral graphs has increased since 1957, when Collatz and Sinogowitz reported first such cases [2] and the results are scattered that it is not easy to make a comprehensive verification with the respect to posed question even for the graphs reported in the literature. But as long as one can associate a structure with a single family, the members of which increase in size and therefore cannot generate isospectrality within the family, one anticipate that it will be possible to distinguish between isospectral structures using the "characteristic polynomial for the family" and specifying its member. By considering families, rather than individual members we in fact can prune or shorten pending fragments or bridges, and if graphs are nonisomorphic and belong to different families, such prunings or abridgments will disclose differences among the families clearly. It is outside

the scope of this presentation to elaborate and investigate possible complications (if they arise). Here we wanted only to draw attention to the characteristic polynomial as a useful graph invariant, potential of which has not been exhausted. In particular we would like to point to its use in the problem of graph recognition and even graph isomorphism. We do this to refute the view that the characteristic polynomials as a tool for such task failed, because it could not resolve the problem in a single step. Because a scheme initially doesnot work it should not be abandoned *unless we fully understand why it fails* and find it beyond possible remedy. In case of isospectral graphs much progress has been made, but we still do not know all possible structural factors that cause their occurence and thus cannot completely characterize them. After a proper characterization of isospectrality one may expect characterization of general structures in terms of characteristic polynomial and closely related concepts. Advantages of characteristic polynomial for characterization (partial so far) is its conceptual simplicity.

Acknowledgment. Professor H. Hosoya examined the manuscript and suggested numerous improvements.

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Received January 22/October 18, 1982