

THE FACTORISATION OF CHEMICAL GRAPHS AND THEIR POLYNOMIALS: A SYSTEMATIC STUDY OF CERTAIN TREES

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Abstract

Characteristic polynomials of the set of 284 trees which have 1–12 vertices of valency 1–3 have been examined for possible factors (divisors) using polynomial division. Twenty of these trees are prime in the sense that they contain no other trees in the set as factors. The remaining 264 trees can all be constructed from a subset of 5 trees and a set of 152 non-graphical polynomials. Some of these polynomials exhibit iso- or sub-spectral relationships with acyclic (matching) polynomials of certain cyclic structures. A few cyclic factors of trees are noted briefly. Twenty pairs and one triad of the trees examined are isospectral.

1. Introduction

The search for factors of a polynomial, especially of the characteristic polynomial of a graph, is seductive and intriguing. Common factors suggest structural relationships, and several related families of structures have been noted [1]. These may be a useful means of classification for information storage and retrieval; they may yield simpler or more revealing ways of expressing the polynomial, and they can aid graph recognition. One might also expect that structural relationships of this kind would be reflected in some connectivity related physicochemical properties, although in practice so far this does not appear to be so [2–4].

Another reason to search for factors is that polynomials can be difficult to solve and, because this difficulty tends to increase with size, a decomposition into a product of smaller polynomials can help towards an accurate solution. This is comparatively unimportant for a characteristic polynomial because its zeros can also be obtained as the eigenvalues of an adjacency matrix. For others, such as acyclic (or matching) polynomials however, it could offer a significant advantage.

Whatever the immediate utility of factorisation, the relationships it seems to show are remarkable and worthy of exploration. The characteristic polynomial (CP)

is always expressed here as a linear combination of characteristic polynomials of linear chains. For example, the CPs of pentadienyl and of 2-methylbutadienyl are written as $L(5)$ and $L(5)-L(1)$, respectively. Randić [1,5] has pointed out that chemists have rather neglected this useful and elegant notation, and has put it to good use himself. It has tended to be used only for intermediate calculations, although it has also been used explicitly [6].

In this paper, a graph is not distinguished from its characteristic polynomial (CP). The term graphical factor is used to denote a polynomial factor of a polynomial which itself corresponds to the characteristic polynomial of some other graph. The term non-graphical factor is used to denote a polynomial factor for which no such corresponding structure has been recognised. The latter term is applied even if there is some "artificial" graph with weighted vertices and/or edges which can be drawn to express the characteristic polynomial.

The term factor can itself cause confusion: its use in connection with a number or a polynomial is obvious, but in connection with a graph, the word is often used for a different concept: that of a spanning sub-tree. For factor in the sense used here, the term Front Divisor has been used [7]. Throughout this paper, however, the word factor is used in its general and better known sense in all cases.

Factorisation is an open-ended task unless arbitrary limits are placed on the kinds of factors which are acceptable. For example, when factoring integers one generally restricts the results to those which are products of integers. Here we define the task of factoring chemical graphs and their polynomials as that of extracting one or more graphical factors, leaving a residual polynomial which may or may not be graphical.

Even this is not an easy problem. It is difficult to devise algorithms for deducing factors, and especially to devise ones which will find, and will be known to find, all possible factors of the class defined. Some progress has been made with structures which have an obvious symmetry. King [8] examined a number of polyhedral structures: McClelland [9] devised a useful method for exploiting local symmetries in a molecule, and early work on graphical decompositions, pioneered by Heilbronner [10], often incidentally suggested factors. The recognition of the phenomenon of sub-spectrality was a recognition that common factors occur [2,3,8, 11-14]. More recently, McWorter [15] used the Fröbenius matrix to construct the characteristic polynomial; a method which gives an opportunity for obtaining some factors. Randić and his coworkers developed this, and work by Balasubramanian [16], into a method for factorising trees which they called "ultimate pruning" [17]. This bypasses gradual pruning and starts at once with a 2×2 determinant whose elements are fragments of the initial tree. By choosing alternative forms of the "ultimate determinant", it is possible to see common factors in a row or column, and these will be factors of the original polynomial. This method does not always provide a complete factoring, but it has the considerable advantage over some approaches that the factor-

ing is not necessarily symmetry related. It is though, in its present form, confined to trees.

A recently published paper on the computation of the characteristic polynomial [18] refers to Krylov's method [19]. This sometimes yields a factor of the desired characteristic polynomial, and we wondered if this could form the basis of a method for factoring. However, preliminary trials have not been promising; it is too capricious and unreliable.

We have adopted a less subtle approach to the problem, and in a previous paper [20], the technique of polynomial division was described and a few arbitrarily chosen examples shown. This is simply the division of one polynomial into another to test whether the one is a factor of the other: for if it is, it will leave no remainder. Such an elementary test now has practical use because of two recent developments: (i) the availability of small computers which can be easily programmed to perform the rather tedious task of polynomial division quickly and accurately, and (ii) the discovery of practically useful methods for evaluating the characteristic [21–25] and acyclic [26,27] polynomials.

A fundamental weakness of this method (although it is not alone in this respect) is that there is no assurance of completeness. It will only confirm or reject possible factors that have been considered and thought appropriate to test. On the other hand, modern computer technology makes the extensive testing and searching of lists much more practicable than before. The method is also very powerful in another sense: it is not confined to any particular class of graph (e.g. to trees or polycyclics), nor to any particular kind of polynomial. A final point of interest is that polynomial division appears occasionally to show up the occurrence of a factor that is ignored by other methods [20].

This paper focusses upon a certain set of acyclic structures (trees): those which have 1–12 vertices and valencies in the range 1–3. This particular set was chosen because it includes graphs of conjugated hydrocarbons, and a recent publication [28] provides a complete ordered list of its members. It is also a list of manageable size (284 members) for use with a standard (IBM) personal computer.

2. Method used

2.1. CODING A STRUCTURE FOR COMPUTER USE

Quite a lot of work has been done on the development of efficient codes for computer use, and a recent paper by Balaban et al. [29] gives a useful and up to date review of the subject. Their own method is based on hierarchically ordered extended connectivities.

The numbers in one triangular half of an adjacency matrix provide all the connectivity information required for a code. Since, however, there are $n!$ possible

adjacency matrices for any given structure with n vertices, the code will be more useful if one particular adjacency matrix can be defined. Randić [30–33] chose the one which, when the rows of elements are read sequentially, gives the smallest binary number. Hendrickson and Toczko used a similar scheme but preferred maximal numbering of the adjacency matrix [34]. For trees, the " N -tuple" representation published from Zagreb and Düsseldorf can be used [28]. These all provide a unique code for a particular structure. The N -tuple code can be extended to cyclic structures along lines recently outlined by Randić [35].

Although the N -tuple code is very attractive, and is in principle easy to construct, the author has not found it particularly convenient to use for the typing of extensive lists of structures. This is mainly because it does take time, and it is not always easy immediately to recognise transcription errors. So for practical purposes, in this study we have chosen to forego the benefit of a unique representation in favour of one which is very simple to encode and decode, and which makes immediate use of the information presented. In this method, the n -vertex structure is, by an appropriate numbering, regarded as some deviation from a linear n -vertex system. Only the system size and the connections which define deviations from linearity need to be recorded. The structure so defined is unique. There are many possible codes which could define it with equal validity, but only a few will be of the same minimum length. For these fairly simple structures, it is quite easy to choose a minimal number of fragments by inspection.

2.2. PRACTICAL CODING RULES

Encoding (fig. 1 shows an example):

- (1) Count the (n) vertices and set the first code element to this number.
- (2) If the structure is nonlinear, then break it into as few as possible linear fragments by marking appropriate connections to be broken. It does not matter if the number of linear fragments produced is not minimal, although it will lengthen the code needlessly if it is not.

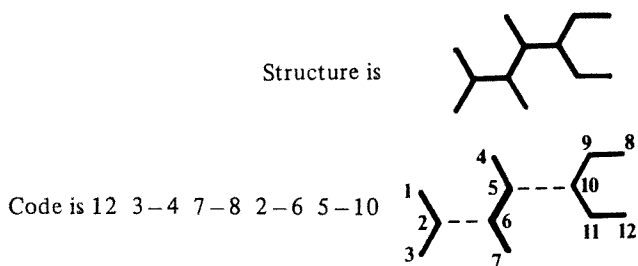


Fig. 1. An example of structure encoding.

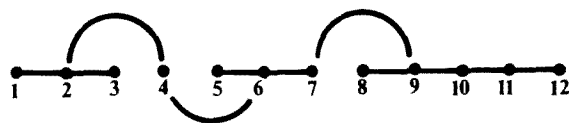
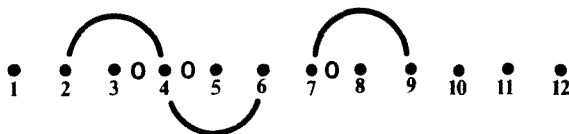
- (3) Number the whole assembly, which forms a disconnected graph, with the vertices of each fragment being numbered consecutively.
- (4) Record each pair of vertices which, in comparison with a consecutively numbered linear chain of n vertices, has a connection made or deleted.

It follows from this description that every code will be an odd length string of numbers. The set of 284 trees considered here can all be encoded with 13 or fewer numbers.

Decoding (fig. 2 shows an example):

- (1) Read the first code element n and draw a sequence of n dots numbered consecutively.
- (2) Read each subsequent pair of numbers. If they are consecutive, then mark the pair of numbered dots as not connected; otherwise draw a connection.

Code is 12 3-4 2-4 4-5 4-6 7-8 7-9



Structure is

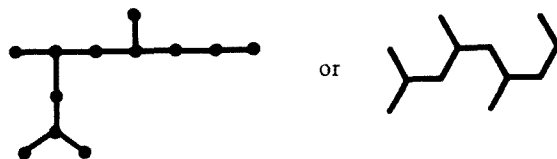


Fig. 2. An example of decoding.

- (3) Draw in the remaining unmarked consecutive connections.
- (4) If necessary, redraw the graph to "straighten" the bonds and give a more conventionally arranged structure.

2.3. DERIVATION OF CHARACTERISTIC POLYNOMIALS

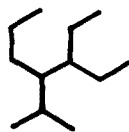
The computer file of 284 structure codes was read by a program which converts each code into the corresponding adjacency matrix, and converts this into its characteristic polynomial using "Frame's method" [21–25,36]. Each characteristic polynomial was stored and manipulated in the form of a string of coefficients which represents a linear combination of characteristic polynomials of linear polyenes. Computer programs are described in refs. [22,24,25]. This method for the characteristic polynomial, which involves a succession of matrix multiplications to give traces which bear a simple relationship to the coefficients, was brought to the attention of chemists by Balasubramanian [21] and ascribed by him to Frame [36]. Recently, Barakat [37] has shown that the so-called Frame's method is "nothing but symmetric functions and Newton's identities". For a comment on the solution of Newton's identities, see Randić's paper [38].

2.4. TESTING BY DIVISION FOR POSSIBLE FACTORS OF POLYNOMIALS

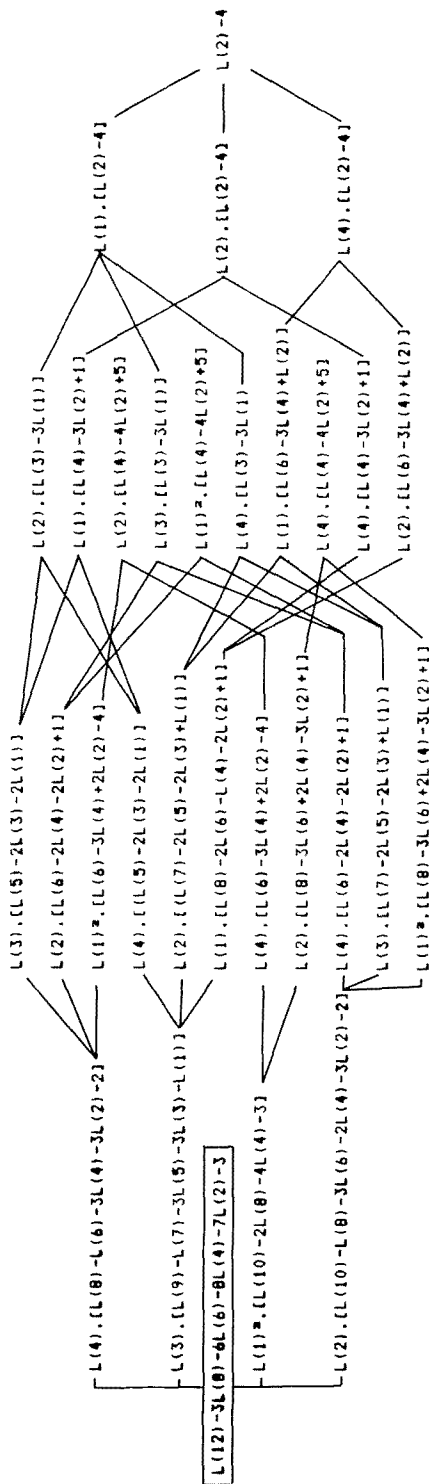
The tool for this work is a program which examines a file of polynomials under test (file A), and against each one it tries each member of a second reference list of possible polynomial factors (file B). If division leaves no remainder, then a factor has been found; it is tried again on the quotient until division fails, and then moves on to try the next possible factor on the original polynomial. Each factor (with its power if it divides more than once), together with the residual polynomial after extraction from the file A polynomial, forms a record in a new file C.

The residual polynomials in file C are examined for duplicates, sorted, and themselves examined for factors in the same way to produce a new file of factors and residual polynomials, and so on. To aid searching and recognition, lists of non-graphical polynomials were sorted each time they were assembled. The list is first grouped in ascending order of n . It is then successively sorted on the basis of the magnitude of each coefficient from $n - 1$ to 0. If this is done, it is easy to search a printed list by eye for a particular polynomial, if required. After a few such iterations, a file of residual polynomials is obtained which do not contain any file B factors. For this particular case, file A and file B start out as being identical, although the entries in file B actually examined can be restricted to those of the same or lower order than the polynomial being divided. A file B polynomial which is of the same order will only show up a factor if it is isospectral (quotient = 1).

For this list of 284 characteristic polynomials, four iterations were needed to fully extract all structural factors. The records in each file were given pointers to enable successive factorisations to be traced through. The combination of these lists of file records can thus be regarded as sets of trees where every path represents a possible factorisation, and where a number of redundancies will occur because a new ordering of factors will be regarded as a new factorisation. This may be illustrated by fig. 3, where the results of the factorisation of structure number 257 are shown.



Structure reference 257; Code 12 3-4 2-7 7-8 7-10



Each product is a factorisation of the right-hand side factor of a product in the preceding column, so that a full factorisation is obtained by tracing a path and recording left-hand side factors together with the last product on the path in full. Ignoring intermediate factorisations, and eliminating repetition caused by a different ordering of factors, this search yields two final products: $L(1) \cdot L(2) \cdot L(3) \cdot L(4) \cdot [L(2) - 4]$ and $L(1)^2 \cdot L(2) \cdot L(4) \cdot [L(4) - 4L(2) + 5]$. The non-graphical polynomial $L(4) - 4L(2) + 5$ can be factored into $[L(2) - 1] \cdot [L(2) - 4]$ and $L(3)$ factorises to $L(1) \cdot [L(2) - 1]$. The most complete factorisation found for this structure is therefore $L(1)^2 \cdot L(2) \cdot L(4) \cdot [L(2) - 1] \cdot [L(2) - 4]$.

Fig. 3. An example of the successive factorisations found by a programmed search.

Although the residual polynomials obtained by this process no longer contain graphical factors, it was found that a number of them are actually products of others in the same list. The first list of 245 residual non-graphical polynomials was therefore tested against itself in a similar manner, and a final "irreducible" list of 152 obtained.

Table 3 shows the final list of factorisations obtained when duplicates are eliminated. The lists shown in tables 1–3 are also available in computer-readable form: see appendix.

3. Discussion

3.1. RESULTS

Table 1 lists all the trees considered (1–12 vertices; valency 1–3) together with their characteristic polynomials. The 284 trees follow the same sequence as is given in ref. [28], but in reverse order for each system size. In the table, each tree is shown as a code, from which its structure can be reconstructed. Within this paper, a given structure is referred to by its list number given in table 1. The methods of calculation used are given in the methods section above.

Table 2 lists the 152 non-graphical polynomial factors which remained when all graphical factors had been extracted from the polynomials of table 1, and table 8 shows those which occur most frequently.

Table 3 shows, as a set of reference numbers, the unique factorisations obtained, each one being the product of one or more graphical factors with one or more non-graphical factors. The graphical factors shown are not all prime, because many of them can themselves be factorised, as can be seen by inspection of the list in table 3. Graphical factors are listed in table 4, and table 7 shows the ten which occur most frequently. Twenty of the polynomials are prime (see below), and are listed in table 5. Of these twenty, fifteen represent trees which could neither be factorised themselves nor used to build other trees. (This last fact has, of course, no significance for the trees of order 12, since that was the largest size examined.)

It follows from table 5 that the ultimate list of graphical factors is quite small and consists of only five polynomials: $L(1)$, $L(2)$, $L(4)$, $L(6)$, and $L(8) - 2L(4) - 3L(2) - 1$. Thus, the table 1 list of 284 characteristic polynomials consists of 20 which are unfactorisable (by the tool applied), plus 264 which can all be expressed as some product from 5 graphical and 152 non-graphical factors.

3.2. PRIME TREES

Prime means (here) not divisible by any of the other trees of table 1. The 20 prime trees found (table 5) do not seem to show any consistent relationships among themselves. Structures 21: $CP = L(8) - L(4) - L(2)$ and 53: $CP = L(10) - L(6) - L(4)$ are an obviously related pair, but the third member of this series [159: $CP = L(12) - L(8) - L(6)$] is factorisable.

All even length chains are prime except for $L(8)$, and this polynomial is an interesting absentee from the list of table 5. Randić et al. [17] state that even length chains have no factors of similar parity. This is not quite correct, for $L(8)$ may be factorised as $L(2) \cdot [L(6) - L(4) + 1]$. It is easy to verify that $L(2)$ is a factor of the series $L(6N + 8)$. The first few members are shown below and form a simple recurrent sequence.

$$\begin{aligned} L(8) &= L(2) \cdot [L(6) - L(4) + 1] \\ L(14) &= L(2) \cdot [L(12) - L(10) + L(6) - L(4) + 1] \\ L(20) &= L(2) \cdot [L(18) - L(16) + L(12) - L(10) + L(6) - L(4) + 1] \\ L(26) &= L(2) \cdot [L(24) - L(22) + L(18) - L(16) + L(12) - L(10) + L(6) - L(4) + 1] \\ L(32) &= L(2) \cdot [L(30) - L(28) + L(24) - L(22) + L(18) - L(16) + L(12) - L(10) + L(6) - L(4) + 1] \end{aligned}$$

If $L(2)$ is regarded as having the notional factorisation $L(2) \cdot (1)$, then the sequence can be generalized to $L(6N + 2)$. This can be shown in algebraic terms:

The division of $L(n)$ by $L(2)$ can be expressed as

$$L(n)/L(2) = L(n-2) - L(n-4) + L(n-6)/L(2),$$

which can be rewritten as

$$L(n+6)/L(2) = L(n+4) - L(n+2) + L(n)/L(2).$$

If $L(2)$ is a factor of $L(n)$, then it is a factor of

$$L(2) \cdot [L(n+4) - L(n+2)] + L(n),$$

which evaluates to $L(n+6)$. Using $n = 2$ for the first factorisable chain gives the recurrent sequence shown.

This extraction of an $L(2)$ factor illustrates the power of this method to show factors which may otherwise be overlooked. In the case of $L(8)$, it is evident from published eigenvalues [39] that $L(2)$ must be a factor, and this fact may also be deduced graphically. If Heilbronner's technique [10] is applied to the second bond of octatetraene, the result $L(8) = L(2) \cdot L(6) - L(1) \cdot L(5)$ is obtained. $L(5)$, pentadienyl, can be seen from its symmetry to have a factor $L(2)$. Therefore, $L(2)$ is a factor of $L(8)$.

3.3. ISOSPECTRAL TREES

Table 6 shows the isospectral trees which occur in the set examined (20 pairs and 1 triad). They are easily detected by the scheme described, for if a tree has an isospectral partner, it will show one factorisation as a single graphical factor reference

Table 1
 Characteristic polynomials of all trees with a maximum of twelve vertices and a maximum valency of three

Structure code*	Characteristic polynomial**
1	$L(1)$
2	$L(2)$
3	$L(3)$
4	$L(4)$
5	$L(4) - 1$
6	$L(5)$
7	$L(5) - L(1)$
8	$L(6)$
9	$L(6) - L(2) - 1$
10	$L(6) - L(2)$
11	$L(6) - 2L(2) - 1$
12	$L(7)$
13	$L(7) - L(3) - 2L(1)$
14	$L(7) - L(3) - L(1)$
15	$L(7) - L(3)$
16	$L(7) - 2L(3)$
17	$L(7) - 2L(3) - 2L(1)$
18	$L(8)$
19	$L(8) - L(4) - 2L(2) - 1$
20	$L(8) - L(4) - L(2) - 1$
21	$L(8) - L(4) - L(2)$
22	$L(8) - L(4)$
23	$L(8) - 2L(4) + 1$
24	$L(8) - 2L(4) - L(2)$
25	$L(8) - 2L(4) - 3L(2) - 1$
26	$L(8) - 2L(4) - 3L(2) - 2$
27	$L(8) - 2L(4) - 2L(2) - 1$
28	$L(8) - 3L(4) - 3L(2) - 1$
29	$L(9)$
30	$L(9) - L(5) - 2L(3) - 2L(1)$
31	$L(9) - L(5) - 2L(3) - L(1)$
32	$L(9) - L(5) - L(3) - L(1)$

33	9	4-5	2-5				$L(9) - L(5) - L(3)$
34	9	3-4	2-4				$L(9) - L(5)$
35	9	3-4	2-4		6-7	6-8	$L(9) - 2L(5) + L(1)$
36	9	3-4	2-4		5-6	5-7	$L(9) - 2L(5) - L(3) + L(1)$
37	9	4-5	2-5		5-6	5-7	$L(9) - 2L(5) - 2L(3)$
38	9	3-4	2-4		4-5	4-7	$L(9) - 2L(5) - 2L(3) - L(1)$
39	9	3-4	2-4		4-5	4-6	$L(9) - 2L(5) - L(3) - L(1)$
40	9	4-5	2-7				$L(9) - 2L(5) - 4L(3) - 3L(1)$
41	9	4-5	2-6				$L(9) - 2L(5) - 3L(3) - 2L(1)$
42	9	3-4	2-6				$L(9) - 2L(5) - 3L(3) - 3L(1)$
43	9	3-4	2-5				$L(9) - 2L(5) - 2L(3) - L(1)$
44	9	3-4	2-5		6-7	6-8	$L(9) - 3L(5) - 2L(3)$
45	9	3-4	2-6		6-7	6-8	$L(9) - 3L(5) - 4L(3) - 4L(1)$
46	9	3-4	2-5		5-6	5-7	$L(9) - 3L(5) - 4L(3) - 2L(1)$
47	10						$L(10)$
48	10	7-8	4-8				$L(10) - L(6) - 2L(4) - 3L(2) - 1$
49	10	6-7	3-7				$L(10) - L(6) - 2L(4) - 2L(2) - 1$
50	10	6-7	2-7				$L(10) - L(6) - L(4) - L(2) - 1$
51	10	5-6	3-6				$L(10) - L(6) - 2L(4) - L(2)$
52	10	5-6	2-6				$L(10) - L(6) - L(4) - L(2)$
53	10	4-5	2-5				$L(10) - L(6) - L(4)$
54	10	3-4	2-4				$L(10) - L(6) - L(4)$
55	10	3-4	2-4		7-8	7-9	$L(10) - 2L(6) + L(2)$
56	10	3-4	2-4		6-7	6-8	$L(10) - 2L(6) - L(4) + L(2) + 1$
57	10	4-5	2-5		6-7	6-8	$L(10) - 2L(6) - 2L(4) + L(2) + 1$
58	10	3-4	2-4		5-6	5-8	$L(10) - 2L(6) - 2L(4) + 1$
59	10	3-4	2-4		5-6	5-7	$L(10) - 2L(6) - L(4)$
60	10	4-5	2-5		5-6	5-8	$L(10) - 2L(6) - 3L(4) - L(2)$
61	10	4-5	2-5		5-6	5-7	$L(10) - 2L(6) - 2L(4) - L(2)$
62	10	3-4	2-4		4-5	4-7	$L(10) - 2L(6) - 2L(4) - 2L(2) - 1$
63	10	3-4	2-4		4-5	4-6	$L(10) - 2L(6) - L(4) - L(2) - 1$
64	10	3-4	2-4		4-5	4-6	$L(10) - 3L(6) - L(4) - 1$
65	10	5-6	3-8				$L(10) - 2L(6) - 5L(4) - 5L(2) - 2$
66	10	5-6	3-7				$L(10) - 2L(6) - 4L(4) - 4L(2) - 1$
67	10	5-6	2-7				$L(10) - 2L(6) - 3L(4) - 3L(2) - 1$
68	10	4-5	2-7				$L(10) - 2L(6) - 4L(4) - 4L(2) - 2$
69	10	3-4	2-7				$L(10) - 2L(6) - 3L(4) - 4L(2) - 2$
70	10	4-5	2-6				$L(10) - 2L(6) - 3L(4) - 2L(2) - 1$

7-8 7-9

Table 1 (continued)

Structure code*									Characteristic polynomial**
71	10	3-4	2-6						$L(10) - 2L(6) - 3L(4) - 3L(2) - 1$
72	10	3-4	2-5						$L(10) - 2L(6) - 2L(4) - L(2)$
73	10	3-4	2-5	7-8	7-9				$L(10) - 3L(6) - 2L(4) + L(2) + 1$
74	10	4-5	2-6	7-8	7-9				$L(10) - 3L(6) - 3L(4) - L(2)$
75	10	3-4	2-6	7-8	7-9				$L(10) - 3L(6) - 3L(4) - 2L(2) - 1$
76	10	3-4	2-5	6-7	6-8				$L(10) - 3L(6) - 3L(4) + 1$
77	10	3-4	2-7	7-8	7-9				$L(10) - 3L(6) - 4L(4) - 5L(2) - 3$
78	10	3-4	2-4	4-5	4-6	7-8	4-9		$L(10) - 4L(6) - 5L(4) - 6L(2) - 4$
79	10	4-5	2-6	6-7	6-8				$L(10) - 3L(6) - 5L(4) - 3L(2) - 1$
80	10	3-4	2-6	6-7	6-8				$L(10) - 3L(6) - 5L(4) - 5L(2) - 2$
81	10	3-4	2-5	5-6	5-8				$L(10) - 3L(6) - 5L(4) - 4L(2) - 1$
82	10	3-4	2-5	5-6	5-7				$L(10) - 3L(6) - 4L(4) - 3L(2) - 1$
83	10	3-4	2-5	7-8	6-9				$L(10) - 4L(6) - 5L(4) - 2L(2)$
84	11								$L(11)$
85	11	7-8	4-8						$L(11) - L(7) - 2L(5) - 3L(3) - 2L(1)$
86	11	7-8	3-8						$L(11) - L(7) - 2L(5) - 2L(3) - 2L(1)$
87	11	6-7	3-7						$L(11) - L(7) - 2L(5) - 2L(3) - L(1)$
88	11	6-7	2-7						$L(11) - L(7) - L(5) - L(3) - L(1)$
89	11	5-6	3-6						$L(11) - L(7) - 2L(5) - L(3)$
90	11	5-6	2-6						$L(11) - L(7) - L(5) - L(3)$
91	11	4-5	2-5						$L(11) - L(7) - L(5)$
92	11	3-4	2-4						$L(11) - L(7)$
93	11	3-4	2-4	8-9	8-10				$L(11) - 2L(7) + L(3)$
94	11	3-4	2-4	7-8	7-9				$L(11) - 2L(7) - L(5) + L(3) + L(1)$
95	11	4-5	2-5	7-8	7-9				$L(11) - 2L(7) - 2L(5) + L(3) + 2L(1)$
96	11	3-4	2-4	6-7	6-9				$L(11) - 2L(7) - 2L(5) + 2L(1)$
97	11	3-4	2-4	6-7	6-8				$L(11) - 2L(7) - L(5) + L(1)$
98	11	4-5	2-5	6-7	6-9				$L(11) - 2L(7) - 3L(5) + 2L(1)$
99	11	4-5	2-5	6-7	6-8				$L(11) - 2L(7) - 2L(5) + L(1)$
100	11	3-4	2-4	5-6	5-8				$L(11) - 2L(7) - 2L(5) - L(3)$
101	11	3-4	2-4	5-6	5-7				$L(11) - 2L(7) - L(5) - L(1)$
102	11	5-6	3-6	6-7	6-9				$L(11) - 2L(7) - 4L(5) - 2L(3)$
103	11	5-6	3-6	6-7	6-8				$L(11) - 2L(7) - 3L(5) - 2L(3)$

104	11	5-6	2-6	6-7	6-8	$L(11) - 2L(7) - 2L(5) - 2L(3)$
105	11	4-5	2-5	5-6	5-8	$L(11) - 2L(7) - 3L(5) - 2L(3) - L(1)$
106	11	3-4	2-4	4-5	4-8	$L(11) - 2L(7) - 2L(5) - 3L(3) - 2L(1)$
107	11	4-5	2-5	5-6	5-7	$L(11) - 2L(7) - 2L(5) - L(3) - L(1)$
108	11	3-4	2-4	4-5	4-7	$L(11) - 2L(7) - 2L(5) - 2L(3) - 2L(1)$
109	11	3-4	2-4	4-5	4-6	$L(11) - 2L(7) - L(5) - L(3) - L(1)$
110	11	3-4	2-4	4-5	4-6	$L(11) - 3L(7) - L(5) + L(3) - L(1)$
111	11	3-4	2-4	4-5	4-7	$L(11) - 3L(7) - 2L(5) - L(3) - 2L(1)$
112	11	3-4	2-4	4-5	4-6	$L(11) - 3L(7) - 2L(5)$
113	11	5-6	3-8			$L(11) - 2L(7) - 5L(5) - 6L(3) - 4L(1)$
114	11	5-6	2-8			$L(11) - 2L(7) - 4L(5) - 5L(3) - 3L(1)$
115	11	4-5	2-8			$L(11) - 2L(7) - 4L(5) - 5L(3) - 4L(1)$
116	11	5-6	3-7			$L(11) - 2L(7) - 4L(5) - 4L(3) - 2L(1)$
117	11	5-6	2-7			$L(11) - 2L(7) - 3L(5) - 3L(3) - 2L(1)$
118	11	4-5	2-7			$L(11) - 2L(7) - 4L(5) - 4L(3) - 3L(1)$
119	11	3-4	2-7			$L(11) - 2L(7) - 3L(5) - 4L(3) - 3L(1)$
120	11	4-5	2-6			$L(11) - 2L(7) - 3L(5) - 2L(3) - L(1)$
121	11	3-4	2-6			$L(11) - 2L(7) - 3L(5) - 3L(3) - L(1)$
122	11	3-4	2-5			$L(11) - 2L(7) - 2L(5) - L(3)$
123	11	3-4	2-5	8-9	8-10	$L(11) - 3L(7) - 2L(5) + L(3) + 2L(1)$
124	11	4-5	2-6	8-9	8-10	$L(11) - 3L(7) - 3L(5) + L(1)$
125	11	3-4	2-6	8-9	8-10	$L(11) - 3L(7) - 3L(5) - L(3) + L(1)$
126	11	3-4	2-5	7-8	7-9	$L(11) - 3L(7) - 3L(5) + L(3) + 3L(1)$
127	11	5-6	3-7	8-9	8-10	$L(11) - 3L(7) - 4L(5) - 3L(3)$
128	11	5-6	2-7	8-9	8-10	$L(11) - 3L(7) - 3L(5) - 2L(3) - L(1)$
129	11	4-5	2-7	8-9	8-10	$L(11) - 3L(7) - 4L(5) - 3L(3) - 2L(1)$
130	11	3-4	2-7	8-9	8-10	$L(11) - 3L(7) - 3L(5) - 3L(3) - 3L(1)$
131	11	4-5	2-6	7-8	7-9	$L(11) - 3L(7) - 4L(5) - L(3) + L(1)$
132	11	3-4	2-6	7-8	7-9	$L(11) - 3L(7) - 4L(5) - 2L(3)$
133	11	3-4	2-5	6-7	6-9	$L(11) - 3L(7) - 4L(5) - L(3) + 2L(1)$
134	11	3-4	2-5	6-7	6-8	$L(11) - 3L(7) - 3L(5) - L(3) + L(1)$
135	11	3-4	2-5	8-9	7-10	$L(11) - 4L(7) - 4L(5) + L(3) + 4L(1)$
136	11	3-4	2-8	8-9	8-10	$L(11) - 3L(7) - 4L(5) - 5L(3) - 4L(1)$
137	11	3-4	2-4	5-6	5-7	$L(11) - 4L(7) - 4L(5) - 3L(3) - 4L(1)$
138	11	4-5	2-7	7-8	7-9	$L(11) - 3L(7) - 6L(5) - 6L(3) - 4L(1)$
139	11	3-4	2-7	7-8	7-9	$L(11) - 3L(7) - 5L(5) - 6L(3) - 5L(1)$
140	11	3-4	2-4	4-5	4-6	$L(11) - 4L(7) - 6L(5) - 7L(3) - 6L(1)$

8-9 8-10
8-9 8-10
7-8 7-9

8-9 4-10

7-8 4-9

Table 1 (continued)

Structure code*					Characteristic polynomial**	
141	11	4-5	2-6	6-7	6-9	$L(11) - 3L(7) - 6L(5) - 5L(3) - 2L(1)$
142	11	3-4	2-6	6-7	6-9	$L(11) - 3L(7) - 6L(5) - 7L(3) - 4L(1)$
143	11	4-5	2-6	6-7	6-8	$L(11) - 3L(7) - 5L(5) - 4L(3) - 2L(1)$
144	11	3-4	2-6	6-7	6-8	$L(11) - 3L(7) - 5L(5) - 6L(3) - 3L(1)$
145	11	3-4	2-5	5-6	5-8	$L(11) - 3L(7) - 5L(5) - 5L(3) - 3L(1)$
146	11	3-4	2-5	5-6	5-7	$L(11) - 3L(7) - 4L(5) - 3L(3) - 2L(1)$
147	11	3-4	2-5	7-8	6-8	$L(11) - 4L(7) - 4L(5) - L(3)$
148	11	3-4	2-5	8-9	6-10	$L(11) - 4L(7) - 6L(5) - 5L(3) - 2L(1)$
149	11	3-4	2-5	7-8	6-9	$L(11) - 4L(7) - 6L(5) - 3L(3)$
150	12					$L(12)$
151	12	8-9	4-9			$L(12) - L(8) - 2L(6) - 3L(4) - 3L(2) - 1$
152	12	7-8	4-8			$L(12) - L(8) - 2L(6) - 3L(4) - 2L(2) - 1$
153	12	7-8	3-8			$L(12) - L(8) - 2L(6) - 2L(4) - 2L(2) - 1$
154	12	7-8	2-8			$L(12) - L(8) - L(6) - L(4) - L(2) - 1$
155	12	6-7	3-7			$L(12) - L(8) - 2L(6) - 2L(4) - L(2)$
156	12	6-7	2-7			$L(12) - L(8) - L(6) - L(4) - L(2)$
157	12	5-6	3-6			$L(12) - L(8) - 2L(6) - L(4)$
158	12	5-6	2-6			$L(12) - L(8) - L(6) - L(4)$
159	12	4-5	2-5			$L(12) - L(8) - L(6)$
160	12	3-4	2-4			$L(12) - L(8)$
161	12	3-4	2-4	9-10	9-11	$L(12) - 2L(8) + L(4)$
162	12	3-4	2-4	8-9	8-10	$L(12) - 2L(8) - L(6) + L(4) + L(2)$
163	12	4-5	2-5	8-9	8-10	$L(12) - 2L(8) - 2L(6) + L(4) + 2L(2) + 1$
164	12	3-4	2-4	7-8	7-10	$L(12) - 2L(8) - 2L(6) + 2L(2) + 1$
165	12	3-4	2-4	7-8	7-9	$L(12) - 2L(8) - L(6) + L(2) + 1$
166	12	4-5	2-5	7-8	7-10	$L(12) - 2L(8) - 3L(6) + 3L(2) + 2$
167	12	4-5	2-5	7-8	7-9	$L(12) - 2L(8) - 2L(6) + 2L(2) + 1$
168	12	3-4	2-4	6-7	6-9	$L(12) - 2L(8) - 2L(6) - L(4) + L(2) + 1$
169	12	3-4	2-4	6-7	6-8	$L(12) - 2L(8) - L(6)$
170	12	5-6	3-6	7-8	7-10	$L(12) - 2L(8) - 4L(6) - L(4) + 3L(2) + 2$
171	12	5-6	3-6	7-8	7-9	$L(12) - 2L(8) - 3L(6) - L(4) + 2L(2) + 1$
172	12	5-6	2-6	7-8	7-9	$L(12) - 2L(8) - 2L(6) - L(4) + L(2) + 1$
173	12	4-5	2-5	6-7	6-9	$L(12) - 2L(8) - 3L(6) - L(4) + L(2) + 1$

Table 1 (continued)

Structure code*		Characteristic polynomial**
211	12 4-5 2-6	$L(12) - 2L(8) - 3L(6) - 2L(4) - L(2)$
212	12 3-4 2-6	$L(12) - 2L(8) - 3L(6) - 3L(4) - L(2)$
213	12 3-4 2-5	$L(12) - 2L(8) - 2L(6) - L(4)$
214	12 3-4 2-5	$L(12) - 3L(8) - 2L(6) + L(4) + 2L(2) + 1$
215	12 4-5 2-6	$L(12) - 3L(8) - 3L(6) + 2L(2) + 1$
216	12 3-4 2-6	$L(12) - 3L(8) - 3L(6) - L(4) + 2L(2) + 2$
217	12 3-4 2-5	$L(12) - 3L(8) - 3L(6) + L(4) + 4L(2) + 2$
218	12 5-6 3-7	$L(12) - 3L(8) - 4L(6) - 2L(4) + L(2) + 1$
219	12 5-6 2-7	$L(12) - 3L(8) - 3L(6) - L(4)$
220	12 4-5 2-7	$L(12) - 3L(8) - 4L(6) - 2L(4) - L(2)$
221	12 3-4 2-7	$L(12) - 3L(8) - 4L(6) + 3L(2) + 2$
222	12 4-5 2-6	$L(12) - 3L(8) - 4L(6) - L(4) + 3L(2) + 2$
223	12 3-4 2-6	$L(12) - 3L(8) - 4L(6) - L(4) + 3L(2) + 2$
224	12 3-4 2-5	$L(12) - 3L(8) - 4L(6) + 5L(2) + 3$
225	12 3-4 2-5	$L(12) - 3L(8) - 3L(6) + 3L(2) + 2$
226	12 3-4 2-5	$L(12) - 4L(8) - 4L(6) + 2L(4) + 7L(2) + 4$
227	12 6-7 3-8	$L(12) - 3L(8) - 4L(6) - 4L(4) - 2L(2)$
228	12 6-7 2-8	$L(12) - 3L(8) - 3L(6) - 2L(4) - 2L(2) - 1$
229	12 3-4 2-4 6-7 5-8	$L(12) - 4L(8) - 3L(6) - L(2) - 1$
230	12 5-6 3-8	$L(12) - 3L(8) - 5L(6) - 5L(4) - 3L(2) - 1$
231	12 5-6 2-8	$L(12) - 3L(8) - 4L(6) - 4L(4) - 3L(2) - 1$
232	12 4-5 2-8	$L(12) - 3L(8) - 4L(6) - 4L(4) - 4L(2) - 2$
233	12 3-4 2-8	$L(12) - 3L(8) - 3L(6) - 3L(4) - 4L(2) - 2$
234	12 3-4 2-8	$L(12) - 4L(8) - 3L(6) - L(4) - 4L(2) - 3$
235	12 5-6 3-7 8-9	$L(12) - 3L(8) - 5L(6) - 3L(4) + L(2) + 1$
236	12 4-5 2-7 8-9	$L(12) - 3L(8) - 4L(6) - 2L(4)$
237	12 4-5 2-7 8-9	$L(12) - 3L(8) - 5L(6) - 3L(4) - L(2)$
238	12 3-4 2-7 8-9	$L(12) - 3L(8) - 4L(6) - 3L(4) - 2L(2) - 1$
239	12 4-5 2-6 7-8	$L(12) - 3L(8) - 5L(6) - 2L(4) + 2L(2) + 2$
240	12 3-4 2-6 7-8	$L(12) - 3L(8) - 5L(6) - 3L(4) + L(2) + 1$
241	12 4-5 2-6 7-8	$L(12) - 3L(8) - 4L(6) - 2L(4) + L(2) + 1$
242	12 3-4 2-6 7-8	$L(12) - 3L(8) - 4L(6) - 3L(4) + 1$
243	12 3-4 2-5 6-7	$L(12) - 3L(8) - 4L(6) - 2L(4) + L(2) + 1$

244	12	3	4	2	5	6	7	6	8	9	10	9	11	$L(12) - 3L(8) - 3L(6) - L(4)$
245	12	3	4	2	5	6	7	6	8	9	10	9	11	$L(12) - 4L(8) - 3L(6) + L(4) + 2L(2) + 1$
246	12	3	4	2	5	9	10	7	11					$L(12) - 4L(8) - 5L(6) - L(4) + 4L(2) + 3$
247	12	3	4	2	5	8	9	7	10					$L(12) - 4L(8) - 5L(6) + 5L(2) + 3$
248	12	3	4	2	9	9	10	9	11					$L(12) - 3L(8) - 4L(6) - 5L(4) - 4L(2) - 1$
249	12	3	4	2	9	6	7	5	7	9	10	9	11	$L(12) - 4L(8) - 4L(6) - 2L(4) - L(2)$
250	12	3	4	2	9	7	8	5	8	9	10	9	11	$L(12) - 4L(8) - 5L(6) - 3L(4) - 2L(2) - 1$
251	12	4	5	2	8	8	9	8	10					$L(12) - 3L(8) - 6L(6) - 7L(4) - 7L(2) - 3$
252	12	3	4	2	8	8	9	8	10					$L(12) - 3L(8) - 5L(6) - 6L(4) - 6L(2) - 3$
253	12	3	4	2	8	6	7	5	7	8	9	8	10	$L(12) - 4L(8) - 5L(6) - 4L(4) - 5L(2) - 3$
254	12	3	4	2	8	7	8	5	8	8	9	8	10	$L(12) - 4L(8) - 7L(6) - 8L(4) - 8L(2) - 4$
255	12	5	6	3	7	7	8	7	10					$L(12) - 3L(8) - 7L(6) - 7L(4) - 3L(2) - 1$
256	12	4	5	2	7	7	8	7	10					$L(12) - 3L(8) - 7L(6) - 8L(4) - 6L(2) - 2$
257	12	3	4	2	7	7	8	7	10					$L(12) - 3L(8) - 6L(6) - 8L(4) - 7L(2) - 3$
258	12	3	4	2	7	6	7	5	7	7	8	7	10	$L(12) - 4L(8) - 7L(6) - 9L(4) - 8L(2) - 3$
259	12	5	6	3	7	7	8	7	9					$L(12) - 3L(8) - 6L(6) - 6L(4) - 3L(2) - 1$
260	12	5	6	2	7	7	8	7	9					$L(12) - 3L(8) - 5L(6) - 5L(4) - 3L(2) - 1$
261	12	4	5	2	7	7	8	7	9					$L(12) - 3L(8) - 6L(6) - 7L(4) - 5L(2) - 2$
262	12	3	4	2	7	7	8	7	9					$L(12) - 3L(8) - 5L(6) - 7L(4) - 6L(2) - 2$
263	12	3	4	2	7	6	7	5	7	7	8	7	9	$L(12) - 4L(8) - 6L(6) - 8L(4) - 7L(2) - 2$
264	12	4	5	2	6	6	7	6	9					$L(12) - 3L(8) - 6L(6) - 6L(4) - 4L(2) - 1$
265	12	3	4	2	6	6	7	6	9					$L(12) - 3L(8) - 6L(6) - 8L(4) - 6L(2) - 2$
266	12	3	4	2	5	5	6	5	9					$L(12) - 3L(8) - 5L(6) - 6L(4) - 5L(2) - 2$
267	12	4	5	2	6	6	7	6	8					$L(12) - 3L(8) - 5L(6) - 4L(4) - 3L(2) - 1$
268	12	3	4	2	6	6	7	6	8					$L(12) - 3L(8) - 5L(6) - 6L(4) - 4L(2) - 1$
269	12	3	4	2	5	5	6	5	8					$L(12) - 3L(8) - 5L(6) - 5L(4) - 4L(2) - 2$
270	12	3	4	2	5	5	6	5	7					$L(12) - 3L(8) - 4L(6) - 3L(4) - 2L(2) - 1$
271	12	3	4	2	5	7	8	6	8	9	10	9	11	$L(12) - 4L(8) - 4L(6) + L(2)$
272	12	4	5	2	6	8	9	7	9	9	10	9	11	$L(12) - 4L(8) - 5L(6) - 2L(4)$
273	12	3	4	2	6	8	9	7	9	9	10	9	11	$L(12) - 4L(8) - 5L(6) - 4L(4) - L(2) + 1$
274	12	3	4	2	5	8	9	6	9	9	10	9	11	$L(12) - 4L(8) - 5L(6) - 3L(4) - 2L(2) - 1$
275	12	3	4	2	5	7	8	6	8	8	9	8	10	$L(12) - 4L(8) - 5L(6) - L(4) + 2L(2) + 1$
276	12	3	4	2	6	9	10	7	11					$L(12) - 4L(8) - 7L(6) - 8L(4) - 5L(2) - 1$
277	12	3	4	2	5	9	10	6	11					$L(12) - 4L(8) - 6L(6) - 6L(4) - 5L(2) - 2$
278	12	3	4	2	5	6	7	6	8	9	10	6	11	$L(12) - 5L(8) - 7L(6) - 6L(4) - 5L(2) - 2$
279	12	4	5	2	6	8	9	7	10					$L(12) - 4L(8) - 7L(6) - 4L(4) + 1$
280	12	3	4	2	6	8	9	7	10					$L(12) - 4L(8) - 7L(6) - 6L(4) - 2L(2)$

Table 1 (continued)

Structure code [*]	Characteristic polynomial ^{**}
281 12 3-4 2-5 8-9 6-10	$L(12) - 4L(8) - 7L(6) - 6L(4) - 3L(2) - 1$
282 12 3-4 2-5 7-8 6-10	$L(12) - 4L(8) - 7L(6) - 5L(4) + 1$
283 12 3-4 2-5 7-8 6-9	$L(12) - 4L(8) - 6L(6) - 4L(4) - L(2)$
284 12 3-4 2-5 7-8 6-9 9-10 9-11	$L(12) - 5L(8) - 7L(6) - 2L(4) + 3L(2) + 2$

^{*}To reconstruct the graph: draw a consecutively numbered linear chain with the number of vertices equal to the first number of code. For each subsequent pair of code numbers, if the numbers are consecutive, delete a connection; if not, make a connection.

^{**} $L(n)$ represents the characteristic polynomial of a linear chain on n vertices.

Table 2

Non-graphical polynomial factors found for the trees of table 1

1	$L(2) - 4$	53	$L(8) - 3L(6) + L(4) + L(2)$
2	$L(2) - 3$	54	$L(8) - 3L(6) + 2L(4) - 4L(2) + 4$
3	$L(2) - 2$	55	$L(8) - 3L(6) + 2L(4) - 3L(2) + 2$
4	$L(2) - 1$	56	$L(8) - 3L(6) + 2L(4) - 2L(2) + 2$
5	$L(4) - 4L(2) + 6$	57	$L(8) - 3L(6) + 2L(4) - 2L(2) + 3$
6	$L(4) - 3L(2)$	58	$L(8) - 3L(6) + 2L(4) - L(2) + 1$
7	$L(4) - 3L(2) + 2$	59	$L(8) - 3L(6) + 2L(4) - L(2) + 2$
8	$L(4) - 3L(2) + 3$	60	$L(8) - 3L(6) + 2L(4) - 1$
9	$L(4) - 2L(2) - 2$	61	$L(8) - 3L(6) + 2L(4)$
10	$L(4) - 2L(2) - 1$	62	$L(8) - 3L(6) + 3L(4) - 4L(2) + 5$
11	$L(4) - 2L(2)$	63	$L(8) - 3L(6) + 3L(4) - 3L(2) + 3$
12	$L(4) - 2L(2) + 2$	64	$L(8) - 3L(6) + 3L(4) - 2L(2) + 2$
13	$L(4) - L(2) - 1$	65	$L(8) - 3L(6) + 3L(4) - L(2) - 1$
14	$L(4) - L(2)$	66	$L(8) - 3L(6) + 4L(4) - 5L(2) + 6$
15	$L(6) - 4L(4) + 5L(2) - 6$	67	$L(8) - 2L(6) - 2L(4) + 1$
16	$L(6) - 4L(4) + 5L(2) - 4$	68	$L(8) - 2L(6) - 2L(4) + L(2) + 2$
17	$L(6) - 4L(4) + 5L(2) - 3$	69	$L(8) - 2L(6) - L(4) - L(2) - 1$
18	$L(6) - 4L(4) + 6L(2) - 8$	70	$L(8) - 2L(6) - L(4) - L(2)$
19	$L(6) - 4L(4) + 6L(2) - 6$	71	$L(8) - 2L(6) - L(4) - L(2) + 2$
20	$L(6) - 3L(4) + 2$	72	$L(8) - 2L(6) - L(4)$
21	$L(6) - 3L(4) + L(2) - 2$	73	$L(8) - 2L(6) - L(4) + 2$
22	$L(6) - 3L(4) + L(2) - 1$	74	$L(8) - 2L(6) - L(4) + L(2) + 2$
23	$L(6) - 3L(4) + L(2) + 1$	75	$L(8) - 2L(6) - L(4) + 2L(2) + 2$
24	$L(6) - 3L(4) + L(2) + 3$	76	$L(8) - 2L(6) - 3L(2) + 1$
25	$L(6) - 3L(4) + L(2) + 4$	77	$L(8) - 2L(6) - 2L(2)$
26	$L(6) - 3L(4) + 2L(2) - 3$	78	$L(8) - 2L(6) - L(2) - 1$
27	$L(6) - 3L(4) + 2L(2) - 2$	79	$L(8) - 2L(6) - L(2)$
28	$L(6) - 3L(4) + 2L(2) - 1$	80	$L(8) - 2L(6) - L(2) + 1$
29	$L(6) - 3L(4) + 2L(2) + 1$	81	$L(8) - 2L(6) - 1$
30	$L(6) - 3L(4) + 3L(2) - 3$	82	$L(8) - 2L(6) + 1$
31	$L(6) - 3L(4) + 4L(2) - 5$	83	$L(8) - 2L(6) + L(2)$
32	$L(6) - 2L(4) - 2L(2) - 1$	84	$L(8) - 2L(6) + L(2) + 1$
33	$L(6) - 2L(4) - L(2) - 2$	85	$L(8) - 2L(6) + L(4) - 3L(2) + 2$
34	$L(6) - 2L(4) - L(2) - 1$	86	$L(8) - 2L(6) + L(4) - 2L(2) + 2$
35	$L(6) - 2L(4) - L(2) + 1$	87	$L(8) - 2L(6) + L(4) - L(2)$
36	$L(6) - 2L(4) - 2$	88	$L(8) - 2L(6) + L(4) - L(2) + 2$
37	$L(6) - 2L(4)$	89	$L(8) - 2L(6) + 2L(4) - 3L(2) + 3$
38	$L(6) - 2L(4) + 1$	90	$L(8) - L(6) - 3L(4) - 3L(2) - 1$
39	$L(6) - 2L(4) + 2$	91	$L(8) - L(6) - 3L(4) - 2L(2)$
40	$L(6) - 2L(4) + L(2) - 1$	92	$L(8) - L(6) - 2L(4) - 3L(2) - 2$
41	$L(6) - 2L(4) + 2L(2) - 2$	93	$L(8) - L(6) - 2L(4) - 2L(2)$
42	$L(6) - L(4) - 4L(2) - 3$	94	$L(8) - L(6) - 2L(4) - L(2)$
43	$L(6) - L(4) - 2L(2) - 1$	95	$L(8) - L(6) - 2L(4) + 1$
44	$L(6) - L(4) - L(2) - 1$	96	$L(8) - L(6) - 2L(4) + L(2) + 2$
45	$L(6) - L(4) - L(2)$	97	$L(8) - L(6) - L(4) - L(2) - 1$
46	$L(6) - L(4) - 1$	98	$L(8) - L(6) - L(4) + 1$
47	$L(6) - L(4) + 1$	99	$L(8) - L(6) - L(4) + L(2) + 1$
48	$L(8) - 4L(6) + 6L(4) - 9L(2) + 11$	100	$L(8) - L(6) - L(2)$
49	$L(8) - 4L(6) + 6L(4) - 7L(2) + 7$	101	$L(8) - L(6)$
50	$L(8) - 4L(6) + 7L(4) - 9L(2) + 10$	102	$L(10) - 2L(8) - L(6) - 3L(4) - L(2)$
51	$L(8) - 3L(6) + L(4) - L(2) + 1$	103	$L(10) - 2L(8) - L(6) - 3L(4) + L(2) - 2$
52	$L(8) - 3L(6) + L(4) - L(2) + 2$	104	$L(10) - 2L(8) - L(6) - 2L(4) + L(2) - 1$

Table 2 (continued)

105	$L(10) - 2L(8) - L(6) - L(4) - L(2) - 2$	129	$L(10) - 2L(8) + 2L(6) - 2L(4) + 2L(2) - 2$
106	$L(10) - 2L(8) - L(6) - L(4) + L(2) - 1$	130	$L(10) - L(8) - 3L(6) - 3L(4) - 2L(2) - 1$
107	$L(10) - 2L(8) - L(6) - L(4) + 3L(2)$	131	$L(10) - L(8) - 3L(6) - 3L(4)$
108	$L(10) - 2L(8) - L(6) + 3L(2) + 1$	132	$L(10) - L(8) - 3L(6) - 2L(4) - L(2) - 1$
109	$L(10) - 2L(8) - 4L(4) - 2$	133	$L(10) - L(8) - 3L(6) - L(4) + 2L(2) + 1$
110	$L(10) - 2L(8) - 3L(4) - 1$	134	$L(10) - L(8) - 2L(6) - 3L(4) - 2L(2) - 1$
111	$L(10) - 2L(8) - 2L(4) - 2$	135	$L(10) - L(8) - 2L(6) - 3L(4) - L(2) - 1$
112	$L(10) - 2L(8) - 2L(4)$	136	$L(10) - L(8) - 2L(6) - 2L(4) - 2L(2) - 1$
113	$L(10) - 2L(8) - 2L(4) + 2L(2) - 2$	137	$L(10) - L(8) - 2L(6) - 2L(4) - L(2) - 1$
114	$L(10) - 2L(8) - L(4) - L(2) - 1$	138	$L(10) - L(8) - 2L(6) - 2L(4)$
115	$L(10) - 2L(8) - L(4) - 1$	139	$L(10) - L(8) - 2L(6) - 2L(4) + L(2)$
116	$L(10) - 2L(8) - L(4) + L(2) - 2$	140	$L(10) - L(8) - 2L(6) - L(4) - L(2) - 1$
117	$L(10) - 2L(8) - L(4) + L(2) + 1$	141	$L(10) - L(8) - 2L(6) - L(4)$
118	$L(10) - 2L(8) - L(4) + 2L(2) - 1$	142	$L(10) - L(8) - 2L(6) - L(2) - 2$
119	$L(10) - 2L(8) - L(4) + 3L(2) - 1$	143	$L(10) - L(8) - 2L(6) - 1$
120	$L(10) - 2L(8) - 1$	144	$L(10) - L(8) - 2L(6) + L(2)$
121	$L(10) - 2L(8) + L(2) - 1$	145	$L(10) - L(8) - 2L(6) + 2L(2) + 1$
122	$L(10) - 2L(8) + L(6) - 3L(4) + 2L(2) - 2$	146	$L(10) - L(8) - L(6) - 2L(4) - L(2) - 1$
123	$L(10) - 2L(8) + L(6) - 2L(4) - 1$	147	$L(10) - L(8) - L(6) - 2L(4) - 1$
124	$L(10) - 2L(8) + L(6) - 2L(4) + 2L(2) - 3$	148	$L(10) - L(8) - L(6) - L(4)$
125	$L(10) - 2L(8) + L(6) - 2L(4) + 2L(2) - 1$	149	$L(10) - L(8) - L(6) - L(2) - 1$
126	$L(10) - 2L(8) + L(6) - L(4)$	150	$L(10) - L(8) - L(6)$
127	$L(10) - 2L(8) + L(6) - L(4) + L(2) - 2$	151	$L(10) - L(8) - L(6) + L(4) - 1$
128	$L(10) - 2L(8) + L(6) - L(4) + 2L(2) - 2$	152	$L(10) - L(8) - L(4) + L(2) - 1$

$L(n)$ denotes the characteristic polynomial of a linear polyene with n vertices.

Table 3
Factorisations found for the trees of table 1

Structure number (table 1)	Factors*		Structure number (table 1)	Factors*	
	Graphical (table 1)	Non-graphical (table 2)		Graphical (table 1)	Non-graphical (table 2)
1	1		36	1	98
2	2		37	1 4	11
3	1	4	38	1 2	38
4	4		39	1 1 1	31
5	1 1	3	40	2 3	10
6	1 2	3	40	1 2	4 10
7	1	14	41	1 2	37
8	8		42	3	43
9	2	13	42	1	4 43
10	1 1	12	43	1 2	38
11	1 1 2	2	44	1 1 1	30
12	7	4	45	1 1 3	7
12	3	14	45	1 1 1	4 7
12	1	4 14	46	1	93
13	1 2 2	2	47	47	
14	1	46	48	27	4
15	3	13	48	3 3	11
15	1	4 13	48	1 1	4 4 11
16	1 1 3	2	49	49	
16	1 1 1	2 4	50	4	45
17	1	44	51	2 2	39
18	2	47	52	1 1	89
19	2	45	53	53	
20	11	4	54	1 14	3
20	1 2 3	2	54	5	46
20	1 1 2	2 4	54	1 1	3 46
21	21		55	1 1 8	2
22	1 1	41	56	1 1	88
23	1 1 4	2	57	2	96
24	1 1	40	58	1 6	11
25	25		58	2 5	11
26	1 1 2	8	58	1 1 2	3 11
27	1 3	11	59	1 17	3
27	1 1	4 11	59	5	44
28	1 3	10	59	1 1	3 44
28	1 1	4 10	60	2	95
29	1 4	12	61	1 1	86
30	17	4	62	1 1 4	8
30	3	44	63	1 1	87
30	1	4 44	64	1 1 5	8
31	1 2	40	64	1 1 1 1	3 8
32	1	100	65	2 2	35
33	1 2 4	2	66	1 1 2 2	5
34	1	101	67	1 1	85
35	1 11	3	68	68	
35	1 1 6	2	69	28	4
35	1 2 5	2	69	3 3	10
35	1 1 1 2	2 3	69	1 1	4 4 10

Table 3 (continued)

Structure number (table 1)	Factors*			Structure number (table 1)	Factors*					
	Graphical (table 1)	Non-graphical (table 2)			Graphical (table 1)	Non-graphical (table 2)				
70	4			93	1	1	1	2	4	14
71	1	1		94	7			45		
72	1	1		94	1			14	45	
73	1	1		95	17			14		
74	1	1		95	7			44		
75	1	1		95	1			14	44	
76	1	6		96	1	2		83		
76	2	5		97	1	1	1	66		
76	1	1	2	98	1	2	2	29		
77	3	3		99	1	8		11		
77	1	1		100	1			148		
78	1	1	3	101	3			96		
78	1	1	1	101	1			4	96	
79	2	4		102	2	6		10		
80	1	1		102	1	2	2	3	10	
81	1	1	2	103	6			43		
82	1	1	4	103	1	2		3	43	
83	1	1	2	104	1	26		3		
84	2	15		104	1	1	6	8		
84	3	9		104	1	2	5	8		
84	1	9		104	1	1	1	2	3	8
84	6			105	1			147		
84	2	3		106	44			4		
84	1	2		106	1	1	3	30		
85	43			106	1	1	1	4	30	
85	38			107	1	25		3		
85	2	3		108	3			95		
85	1	2		108	1			4	95	
86	37			109	1	27		3		
86	3	4		109	3	5		11		
86	1	4		109	1	5		4	11	
87	1	2		109	1	1	3	3	11	
88	36			109	1	1	1	3	4	11
88	3			110	1	1	3	29		
88	1			110	1	1	1	4	29	
89	2	17		111	1	28		3		
89	6			111	3	5		10		
89	1	2		111	1	5		4	10	
90	1	19		111	1	1	3	3	10	
90	6			111	1	1	1	3	4	10
90	1	2		112	1	1	1	63		
91	1			113	1	2		77		
92	3			114	1	2		78		
92	1			115	46			4		
93	16			115	3			93		
93	1	1	12	115	1			4	93	
93	1	3	7	116	1	2		79		
93	1	1	7	117	1			146		
93	1	1	3	118	1	4		36		

Table 3 (continued)

Structure number (table 1)	Factors*			Structure number (table 1)	Factors*		
	Graphical (table 1)	Non-graphical (table 2)			Graphical (table 1)	Non-graphical (table 2)	
119	3		94	153	2		149
119	1		4 94	154	1 31		3
120	1		147	154	2 24		3
121	1 2		81	154	1 6		40
122	1		148	154	2 5		40
123	1 1 7		8	154	1 1 2		3 40
123	1 1 1		8 14	155	155		
124	1 8		10	156	156		
125	1 1 1		62	157	2		150
126	7		43	158	56		4
126	1		14 43	158	1 3		88
127	1 1 6		7	158	1 1		4 88
127	1 2 5		7	159	2		151
127	1 1 1 2		3 7	160	1 1		129
128	1 5		36	161	1 1 18		2
128	1 1 1		3 36	161	11		47
129	1		137	161	1 1 2		2 27
130	1 1 3		28	162	1 1		128
130	1 1 1		4 28	163	163		
131	1		139	164	1 1 2		64
132	1		138	165	1 3		84
133	1 2 2		24	165	1 1		4 84
134	1 1 1		62	166	2		145
135	1 1 7		7	167	1 1 2		64
135	1 1 1		7 14	168	1 1		125
136	1 1 3		27	169	1 1 2		65
136	1 1 1		4 27	170	2 2 2		25
137	1 1 3		23	171	26		14
137	1 1 1		4 23	171	1 2 7		8
138	1 4		33	171	1 1 2		8 14
139	3		91	172	1 1		125
139	1		4 91	173	2		144
140	1 1 3		22	174	73		4
140	1 1 1		4 22	174	1 3		82
141	1 2 2		23	174	1 1		4 82
142	1 2		69	175	175		
143	1		135	176	1 1		124
144	1 1 1 2		18	177	1 1		127
145	1		134	178	1 7		38
146	1		137	178	1 1		14 38
147	1 1 1		56	179	2		141
148	1 1 1		54	180	1 1		122
149	1		131	181	76		4
150	150			181	1 40		3
151	4		97	181	2 28		3
152	72		4	181	3 6		10
152	61		4	181	1 6		4 10
152	1 3		86	181	2 5		4 10
152	1 1		4 86	181	1 2 3		3 10

Table 3 (continued)

Structure number (table 1)	Factors*				Structure number (table 1)	Factors*			
	Graphical (table 1)		Non-graphical (table 2)			Graphical (table 1)		Non-graphical (table 2)	
181	1	1	2	3 4 10	208	1	40	3	
182	2			143	208	2	28	3	
183	73			4	208	3	6	10	
183	1	3		82	208	1	6	4	10
183	1	1		4 82	208	2	5	4	10
184	184				208	1	2	3	3 10
185	1	1		123	208	1	1	2	3 4 10
186	1	1		124	209	2		140	
187	1	41		3	210	74		4	
187	1	6		37	210	1	3	80	
187	2	5		37	210	1	1	4	80
187	1	1	2	3 37	211	2		143	
188	1	1		126	212	1	1	122	
189	1	1	1 1	50	213	1	2	3	29
190	1	7		37	213	1	1	2	4 29
190	1	1		14 37	214	1	3	75	
191	1	1		120	214	1	1	4	75
192	1	1		121	215	1	1	118	
193	1	1	1 6	5	216	1	1	117	
193	1	1	2 5	5	217	1	1	119	
193	1	1	1 1 2	3 5	218	1	1	2	58
194	28			14	219	1	3	74	
194	1	12		10	219	1	1	4	74
194	3	7		10	220	1	1	113	
194	1	7		4 10	221	1	2	3	24
194	1	3		10 14	221	1	1	2	4 24
194	1	1		4 10 14	222	222			
195	1	1		116	223	1	1	2	59
196	1	1	2	60	224	2	10	10	
197	1	1	1 3	19	224	1	1	2	10 12
197	1	1	1 1	4 19	225	1	1	2	61
198	4			92	226	1	1	108	
199	81			4	227	1	1	112	
199	1	2	3	27	228	1	1	115	
199	1	1	2	4 27	229	1	1	1 1	49
200	82			4	230	1	6	34	
200	1	3	4	7	230	2	5	34	
200	1	1	4	4 7	230	1	1	2	3 34
201	201				231	3	6	9	
202	2			142	231	1	6	4	9
203	2			136	231	2	5	4	9
204	1	2	3	28	231	1	2	3	3 9
204	1	1	2	4 28	231	1	1	2	3 4 9
205	2	4		35	232	1	1	111	
206	1	1	2 4	5	233	1	1	114	
207	1	6		36	234	1	1	5	27
207	2	5		36	234	1	1	1 1	3 17
207	1	1	2	3 36	235	1	1	2	57
208	76			4	236	1	1	113	

Table 3 (continued)

Structure number (table 1)	Factors*				Structure number (table 1)	Factors*			
	Graphical (table 1)		Non-graphical (table 2)			Graphical (table 1)		Non-graphical (table 2)	
237	237				262	1	3		70
238	1	3		73	262	1	1		4 70
238	1	1		4 73	263	1	1	1 3	15
239	2			133	263	1	1	1 1	4 15
240	1	1	2	57	264	2			132
241	1	1	2	58	265	1	1		109
242	1	1	8	7	266	83			4
243	1	1	2	58	266	1	2	3	23
244	1	3		74	266	1	1	2	4 23
244	1	1		4 74	267	267			
245	1	1	1 3	17	268	1	1		110
245	1	1	1 1	4 17	269	1	3		71
246	1	1	2	53	269	1	1		4 71
247	1	1		107	270	1	3		73
248	1	3		72	270	1	1		4 73
248	1	1		4 72	271	1	12		9
249	1	1	1 3	16	271	3	7		9
249	1	1	1 1	4 16	271	1	7		4 9
250	1	3		68	271	1	3		9 34
250	1	1		4 68	271	1	1		4 9 14
251	4			90	272	1	1		106
252	1	1	4	26	273	1	1	1 1	48
253	1	1		105	274	1	3		68
254	1	1	4	21	274	1	1		4 68
255	1	2	2 6	1	275	1	7		34
255	2	2	2 5	1	275	1	1		14 34
255	1	1	2 2 2	1 3	276	1	1		102
256	2			130	277	1	3		67
257	1	2	3 4	1	277	1	1		4 67
257	1	1	2 4	1 4	278	1	3	5	6
258	1	2	3	20	278	1	1	5	4 6
258	1	1	2	4 20	278	1	1	1 3	3 6
259	1	6		33	278	1	1	1 1	3 4 6
259	2	5		33	279	8			42
259	1	1	2	5 33	280	1	1	2	51
260	1	6		34	281	1	1		103
260	2	5		34	282	1	1	2	52
260	1	1	2	3 34	283	1	1		104
261	1	1	2	55	284	1	7		32
					284	1	1		14 32

A graphical factor is a polynomial which corresponds to one of the trees of table 1; a non-graphical factor is one which does not (table 2). In a few cases, these correspond to certain matching polynomials.

Trees which appear as factors of other trees (in table 3)

1		16		41	
2		17		43	
3		18		44	
4		19		46	
5		24		56	
6		25		61	
7		26		72	
8		27		73	
9		28		74	
10		31		76	
11		36		81	
12		37		82	
14		38		83	
15		40			

Table 5
Trees with no structural factors

These trees of table 1, which in a few cases are factors of other trees, are "prime" in the sense that they contain no other tree factors of this type themselves.



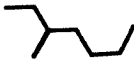
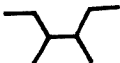

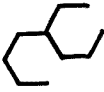
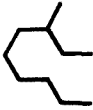
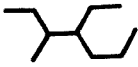

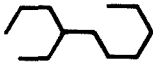
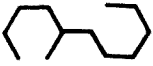
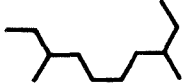
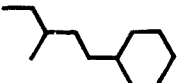
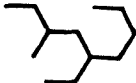
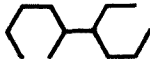
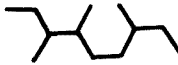
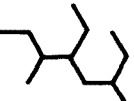
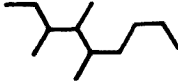
Ref. no. (table 1)	Characteristic polynomial	No. of other trees of table 1, if any, with this factor*	Structure
1	$L(1)$	234	•
2	$L(2)$	97	—
3	$L(4)$	21	
4	$L(6)$	5	
5	$L(8) - L(4) - L(2)$		
6	$L(8) - 2L(4) - 3L(2) - 1$	1	
7	$L(10)$		
8	$L(10) - L(6) - 2L(4) - 2L(2) - 1$		
9	$L(10) - L(6) - L(4)$		
10	$L(10) - 2L(6) - 4L(4) - 4L(2) - 2$		

Table 5 (continued)

Ref. no. (table 1)	Characteristic polynomial	No. of other trees of table 1, if any, with this factor*	Structure
11 150	$L(12)$		
12 155	$L(12) - L(8) - 2L(6) - 2L(4) - L(2)$		
13 156	$L(12) - L(8) - L(6) - L(4) - L(2)$		
14 163	$L(12) - 2L(8) - 2L(6) + L(4) + 2L(2) + 1$		
15 175	$L(12) - 2L(8) - 2L(6)$		
16 184	$L(12) - 2L(8) - 3L(6) - 2L(4) - 2L(2) - 1$		
17 201	$L(12) - 2L(8) - 4L(6) - 5L(4) - 4L(2) - 1$		
18 222	$L(12) - 3L(8) - 4L(6) + 3L(2) + 2$		
19 237	$L(12) - 3L(8) - 5L(6) - 3L(4) - L(2)$		
20 267	$L(12) - 3L(8) - 5L(6) - 4L(4) - 3L(2) - 1$		

*This does not include isospectral partners, which are shown in table 6. The count has no meaning for the 12-vertex trees because this was the largest size examined.

Table 6
Isospectral trees occurring in table 1

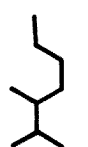
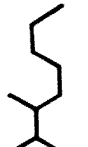
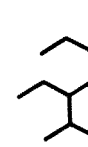
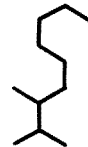
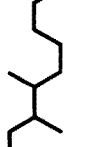
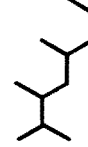
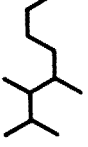
	Ref. nos. (table 1)	Characteristic polynomial and factors found	Structures
1	38 43	$L(9) - 2L(5) - 2L(3) - L(1)$ $= L(1) \cdot L(2) \cdot [L(6) - 2L(4) + 1]$	
2	61 72	$L(10) - 2L(6) - 2L(4) - L(2)$ $= L(1)^2 \cdot [L(8) - 2L(6) + L(4) - 2L(2) + 2]$	
3	67 71	$L(10) - 2L(6) - 3L(4) - 3L(2) - 1$ $= L(1)^2 \cdot [L(8) - 2L(6) + L(4) - 3L(2) + 2]$	
4	100 122	$L(11) - 2L(7) - 2L(5) - L(3)$ $= L(1) \cdot [L(10) - L(8) - L(6) - L(4)]$	
5	105 120	$L(11) - 2L(7) - 3L(5) - 2L(3) - L(1)$ $= L(1) \cdot [L(10) - L(8) - L(6) - 2L(4) - 1]$	
6	125 134	$L(11) - 3L(7) - 3L(5) - L(3) + L(1)$ $= L(1)^3 \cdot [L(8) - 3L(6) + 3L(4) - 4L(2) + 5]$	
7	129 146	$L(11) - 3L(7) - 4L(5) - 3L(3) - 2L(1)$ $= L(1) \cdot [L(10) - L(8) - 2L(6) - 2L(4) - L(2) - 1]$	

Table 6 (continued)

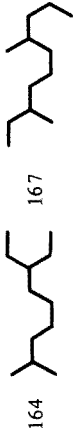
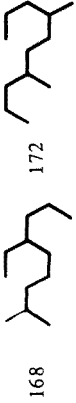
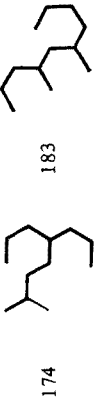
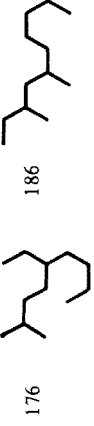
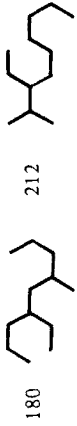
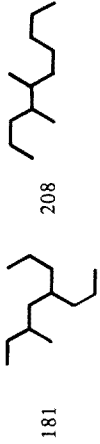
Ref. nos. (table 1)	Characteristic polynomial and factors found	Structures
8 164 167	$L(12) - 2L(8) - 2L(6) + 2L(2) + 1$ $= L(1)^2 \cdot L(2) \cdot [L(8) - 3L(6) + 3L(4) - 2L(2) + 2]$	
9 168 172	$L(12) - 2L(8) - 2L(6) - L(4) + L(2) + 1$ $= L(1)^2 \cdot [L(10) - 2L(8) + L(6) - 2L(4) + 2L(2) - 1]$	
10 174 183	$L(12) - 2L(8) - 2L(6) - 2L(4) - L(2)$ $= L(1)^2 \cdot [L(2) - 1] \cdot [L(8) - 2L(6) + 1]$ $= L(1) \cdot L(3) \cdot [L(8) - 2L(6) + 1]$	
11 176 186	$L(12) - 2L(8) - 2L(6) - L(4) - L(2) - 1$ $= L(1)^2 \cdot [L(10) - 2L(8) + L(6) - 2L(4) + 2L(2) - 3]$	
12 180 212	$L(12) - 2L(8) - 3L(6) - 3L(4) - L(2)$ $= L(1)^2 \cdot [L(10) - 2L(8) + L(6) - 3L(4) + 2L(2) - 2]$	
13 181 208	$L(12) - 2L(8) - 3L(6) - 3L(4) - 2L(2) - 1$ $= [L(10) - 3L(6) - 3L(4) + 1] \cdot [L(2) - 1]$ $= L(1) \cdot [L(9) - 2L(5) - 4L(3) - 3L(1)] \cdot [L(2) - 2]$ $= L(2) \cdot [L(8) - 3L(4) - 3L(2) - 1] \cdot [L(2) - 2]$ $= L(3) \cdot L(5) \cdot [L(4) - 2L(2) - 1]$ $= L(1) \cdot L(5) \cdot [L(2) - 1] \cdot [L(4) - 2L(2) - 1]$ $= L(2) \cdot [L(4) - 1] \cdot [L(2) - 1] \cdot [L(4) - 2L(2) - 1]$ $= L(1) \cdot L(2) \cdot L(3) \cdot [L(2) - 2] \cdot [L(4) - 2L(2) - 1]$ $= L(1)^2 \cdot L(2) \cdot [L(2) - 2] \cdot [L(2) - 1] \cdot [L(4) - 2L(2) - 1]$	

Table 6 (continued)

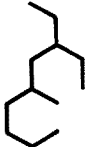
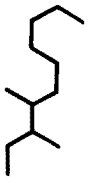

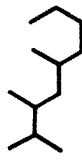
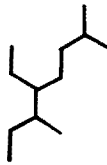
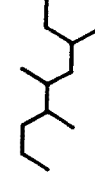
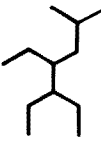
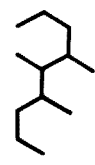
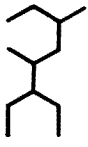
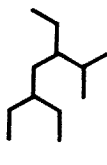
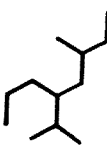
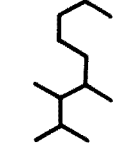
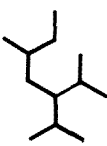
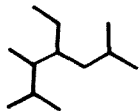


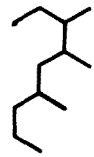
	Ref. nos. (table 1)	Characteristic polynomial and factors found		Structures
14	182 211	$L(12) - 2L(8) - 3L(6) - 2L(4) - L(2)$ $= L(2) \cdot [L(10) - L(8) - 2L(6) - 1]$		 182  211
15	219 244	$L(12) - 3L(8) - 3L(6) - L(4)$ $= L(1)^2 \cdot [L(2) - 1] \cdot [L(8) - 2L(6) - L(4) + L(2) + 2]$ $= L(1) \cdot L(3) \cdot [L(8) - 2L(6) - L(4) + L(2) + 2]$		 219  244
16	220 236	$L(12) - 3L(8) - 4L(6) - 2L(4)$ $= L(1)^2 \cdot [L(10) - 2L(8) - 2L(4) + 2L(2) - 2]$		 220  236
17	230 260	$L(12) - 3L(8) - 5L(6) - 5L(4) - 3L(2) - 1$ $= L(1)^2 \cdot L(2) \cdot [L(2) - 2] \cdot [L(6) - 2L(4) - L(2) - 1]$ $= L(1) \cdot L(5) \cdot [L(6) - 2L(4) - L(2) - 1]$ $= L(2) \cdot [L(4) - 1] \cdot [L(6) - 2L(4) - L(2) - 1]$		 230  260
18	235 240	$L(12) - 3L(8) - 5L(6) - 3L(4) + L(2) + 1$ $= L(1)^2 \cdot L(2) \cdot [L(8) - 3L(6) + 2L(4) - 2L(2) + 3]$		 235  240
19	238 270	$L(12) - 3L(8) - 4L(6) - 3L(4) - 2L(2) - 1$ $= L(1)^2 \cdot [L(2) - 1] \cdot [L(8) - 2L(6) - L(4) + 2]$ $= L(1) \cdot L(3) \cdot [L(8) - 2L(6) - L(4) + 2]$		 238  270

Table 6 (continued)

Ref. nos. (table 1)	Characteristic polynomial and factors found	Structures
20		
250	$L(12) - 4L(8) - 5L(6) - 3L(4) - 2L(2) - 1$ $= L(1)^2 \cdot [L(2) - 1] \cdot [L(8) - 2L(6) - 2L(4) + L(2) + 2]$ $= L(1) \cdot L(3) \cdot [L(8) - 2L(6) - 2L(4) + L(2) + 2]$	 250
274		 274
21		
218	$L(12) - 3L(8) - 4L(6) - 2L(4) + L(2) + 1$ $= L(1)^2 \cdot L(2) \cdot [L(8) - 3L(6) + 2L(4) - L(2) + 1]$	 218
241		 241
243		 243

with a non-graphical factor of 1. (These particular notional factorisations have been eliminated from the list shown in table 3.) All of them factorise to a greater or lesser extent, but factorisation does not appear to be particularly helpful in showing up related structures. The ordinary linear form shows three groups of isospectral pairs which have a similar polynomial form:

$$\begin{array}{lll} 38/43 & 61/72 & 100/122 & L(n) - 2L(n-4) - 2L(n-6) - L(n-8) & \text{for } n = 9 \text{ to } 11 \\ & 67/71 & 180/212 & L(n) - 2L(n-4) - 3L(n-6) - 3L(n-8) - L(n-10) & \text{for } n = 10 \text{ or } 12 \\ & 105/120 & 182/211 & L(n) - 2L(n-4) - 3L(n-6) - 2L(n-8) - L(n-10) & \text{for } n = 11 \text{ or } 12 \end{array}$$

When the first isospectral pair is factorised, it can be seen that it has a similar form to a fourth pair (174/183):

$$\begin{array}{ll} 38/43 & L(1).L(2). [L(6) - 2L(4) + 1] \\ 174/173 & L(1).L(3). [L(8) - 2L(6) + 1]. \end{array}$$

Randić et al. [17] found the same non-graphical factor $L(6) - 2L(4) + 1$ in the isospectral pair of trees 38 and 43. They raise the interesting speculation as to whether this factor is unique. It is not; it is also a factor of structure 85:

$$L(11) - L(7) - 2L(5) - 3L(3) - 2L(1) = L(2).L(3). [L(6) - 2L(4) + 1] ,$$

but this itself contains structure 38/43 as a factor. More significantly, $L(6) - 2L(4) + 1$ is also a factor of 178 which is not related to any of the isospectral pairs:

$$L(12) - 3L(8) - L(6) + 2L(4) - L(2) - 2 = L(1). [L(5) - L(1)]. [L(6) - 2L(4) + 1].$$

Although 38 and 43 form the smallest pair of isospectral trees, $L(6) - 2L(4) + 1$ is not the smallest non-graphical factor which occurs among isospectral trees. $L(2) - 2$ and $L(2) - 1$ are present in some, but only in conjunction with some other non-graphical factor. The smallest non-graphical factor to occur with other factors which are all graphical is $L(4) - 2L(2) - 1$ in the structure pair 181/208:

$$181/208 \quad L(12) - 2L(8) - 3L(6) - 3L(4) - 2L(2) - 1 = L(3).L(5). [L(4) - 2L(2) - 1].$$

(other factorisations are shown in table 6).

This factor also is not unique to isospectral trees.

3.4. THE NATURE OF NON-GRAPHICAL FACTORS OF TREES

Table 2 lists the 152 distinct residual polynomials, all of even order, found in the 284 trees after extracting graphical factors. By definition, none of them can be

Table 7
The most frequently occurring graphical factors

Within table 1, some of the trees, which may or may not be prime, are factors of other trees. The first ten in descending order of frequency are shown here. (See also tables 3 and 4.)









	Ref. no. (table 1)	Characteristic polynomial	No. of trees (besides itself) in which it is a factor	Structure
1	1	$L(1)$	234	•
2	2	$L(2)$	97	—
3	3	$L(3)$	68	
4	4	$L(4)$	21	
5	5	$L(4) - 1$	22	
6	6	$L(5)$	19	
7	7	$L(5) - L(1)$	14	
8	8	$L(6)$	5	
9	28	$L(8) - 3L(4) - 3L(2) - 1$	5	
10	17	$L(7) - 2L(3) - 2L(1)$	4	

Table 8
The most frequently occurring non-graphical factors

"Non-graphical" factors are polynomials (table 2) which are factors of one or more trees in table 1, but which do not represent any of the other trees in table 1. The ten most common are shown here.

	Ref. no. (table 2)	Polynomial	No. of trees in which it is a factor
1	4	$L(2) - 1$	69
2	3	$L(2) - 2$	31
3	14	$L(4) - L(2)$	15
4	10	$L(4) - 2L(2) - 1$	11
5	2	$L(2) - 3$	10
6	11	$L(4) - 2L(2)$	7
7	8	$L(4) - 3L(2) + 3$	6
8	7	$L(4) - 3L(2) + 2$	6
9	27	$L(6) - 3L(4) + 2L(2) - 2$	5
10	44	$L(6) - L(4) - L(2) - 1$	5

The remaining 142 polynomials of table 2 each occur as a factor 1–4 times.

Table 9

Some examples of an iso- or sub-spectral relationship between non-graphical polynomials and the matching polynomials of certain cyclic compounds

Some of the non-graphical polynomials of table 2 are identical or closely related to certain matching polynomials. This is not an exhaustive list because the matching polynomials have not been systematically studied. They are arranged in order of descending frequency of occurrence in the factorisations of table 3








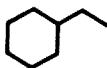




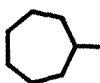
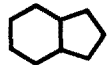


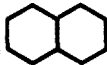



Ref. no. (table 2)	Non-graphical polynomial	A related matching polynomial from structure	Cyclic structure
14	$L(4) - L(2)$	$L(4) - L(2)$	
10	$L(4) - 2L(2) - 1$	$L(4) - 2L(2) - 1$	
11	$L(4) - 2L(2)$	$L(5) - L(3) - 2L(1)$ $= L(1) \cdot [L(4) - 2L(2)]$	
8	$L(4) - 3L(2) + 3$	$L(6) - L(4) - 2L(2)$ $= L(1)^2 \cdot [L(4) - 3L(2) + 3]$	
44	$L(6) - L(4) - L(2) - 1$	$L(6) - L(4) - L(2) - 1$	
9	$L(4) - 2L(2) - 2$	$L(6) - 2L(4) - L(2)$ $= [L(2) - 1] \cdot [L(4) - 2L(2) - 2]$	
34	$L(6) - 2L(4) - L(2) - 1$	$L(6) - 2L(4) - L(2) - 1$	
38	$L(6) - 2L(4) + 1$	$L(8) - L(6) - L(4) - L(2)$ $= L(2) \cdot [L(6) - 2L(4) + 1]$	
45	$L(6) - L(4) - L(2)$	$L(6) - L(4) - L(2)$	
43	$L(6) - L(4) - 2L(2) - 1$	$L(6) - L(4) - 2L(2) - 1$	

Table 9 (continued)

Ref. no. (table 2)	Non-graphical polynomial	A related matching polynomial from	Cyclic structure
12	$L(4) - 2L(2) + 2$	$L(5) - L(3)$ $L(1) \cdot [L(4) - 2L(2) + 2]$	
13	$L(4) - L(2) - 1$	$L(4) - L(2) - 1$	
39	$L(6) - 2L(4) + 2$	$L(8) - L(6) - L(4)$ $= L(2) \cdot [L(6) - 2L(4) + 2]$	
55	$L(8) - 3L(6) + 2L(4) - 3L(2) + 2$	$L(9) - 2L(7) - L(5) - L(3) - L(1)$ $= L(1) \cdot [L(8) - 3L(6) + 2L(4) - 3L(2) + 2]$	
69	$L(8) - 2L(6) - L(4) - L(2) - 1$	$L(8) - 2L(6) - L(4) - L(2) - 1$	
70	$L(8) - 2L(6) - L(4) - L(2)$	$L(8) - 2L(6) - L(4) - L(2)$	
90	$L(8) - L(6) - 3L(4) - 3L(2) - 1$	$L(10) - 2L(8) - L(6) - L(4) - L(2) - 1$ $= [L(2) - 2] \cdot [L(8) - L(6) - 3L(4) - 3L(2) - 1]$	
94	$L(8) - L(6) - 2L(4) - L(2)$	$L(8) - L(6) - 2L(4) - L(2)$	
101	$L(8) - L(6)$	$L(8) - L(6)$	
150	$L(10) - L(8) - L(6)$	$L(10) - L(8) - L(6)$	

represented by any of the graphs considered here. An intriguing property of these polynomials is that some of them are the same as, or are closely related to, the acyclic (or matching) polynomials of certain cyclic or polycyclic structures. Table 9 shows some illustrative examples.

These examples are not exhaustive; they were found by trial and error, without as yet any systematic search of cyclic structure polynomials. They raise two interesting questions. Are all the non-graphical factors found related to some cyclic structure in this way? The answer is probably not, since several of the order four polynomials appear to have no match within the limited range of small cyclic structures, although it might still be the case that they are factors of some larger system. Conversely, is the matching polynomial of a polycyclic structure, or some factor within it, always a factor of some tree? Here again, at first sight the answer appears to be no, because it is easy to find a polycyclic structure whose matching polynomial does not appear in the list of table 2. On the other hand, it has been shown [40,41] that for any cyclic or polycyclic graph, one finds the matching polynomial as a factor of the associated tree introduced by Randić [42] as an auxiliary scheme for counting paths of different lengths. It is likely that the range of graphs considered needs to be enlarged (e.g. to include 4-valent vertices) to find a match, and it is possible that some matching polynomials have not been fully factorised under this brief examination.

A final fascinating and unsolved mathematical problem is this: given a string whose elements represent the coefficients of a linear combination of characteristic polynomials of chains, is it possible to write a generalised string expression which will yield all the polynomials with real zeros, and only those polynomials?

The analysis reported here shows that there are a number of families of related trees whose members are united by a common non-graphical polynomial factor which in some cases can be represented as the acyclic polynomial of some ring-containing structure. Usually, such a family shows regularity in the pattern of its factorised polynomials to a greater or lesser degree and, when there is a well marked pattern, the non-graphical polynomial will occupy a nodal point within the family. Table 10 shows some examples of this.

A corollary of these results is that it is possible to express certain acyclic (matching) polynomials in an unconventional form as a quotient of trees. These polynomials are used to provide a reference for calculating topological resonance energies [43]. This calculation appears to be disliked and mistrusted by some practical chemists on the grounds that the acyclic polynomial is unreal and cannot be visualised. It is problematic whether a quotient of trees can be thought of as any less abstract and "unreal", but if appropriate seeming ratios could be chosen, it might provide the basis for a slightly more helpful notation.


In the case of the simplest cyclic compounds, the annulenes, the acyclic polynomial of an n -membered ring is $L(n) - L(n - 2)$. This can be expressed as the ratio $L(2n - 1)/L(n - 1)$. The acyclic polynomial $[L(6) - L(4)]$ of benzene is thus $L(11)/L(5)$. This polynomial $[L(6) - L(4)]$ does not appear in table 2 because it factorises as $[L(2) - 1] \cdot [L(4) - L(2) - 1]$, but its occurrence as this product may be seen in table 3.


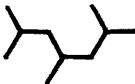
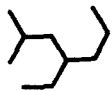
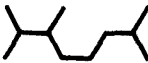
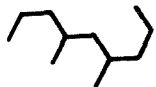
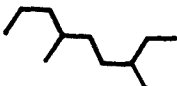
Table 10

Some trees related by common acyclic polynomial factors


This table shows some groups of structures which are united by a common non-graphical factor related to an acyclic (matching) polynomial. In some cases, the polynomial occupies a nodal position in a group which forms a family of structures; in other groups, there is little obvious pattern. The factored forms of characteristic polynomials shown are taken from table 3, and reference numbers refer to table 1 unless noted otherwise.

1. Non-graphical factor $P = L(4) - 3L(2) + 3$ (ref. 8 in table 2)

$L(1)^2 \cdot P$ is the ACYCLIC polynomial of 

26	$L(2) \cdot L(1)^2 \cdot P$		64	$[L(4) - 1] \cdot L(1)^2 \cdot P$	
62	$L(4) \cdot L(1)^2 \cdot P$		123	$[L(5) - L(1)] \cdot L(1)^2 \cdot P$	
104	$L(5) \cdot L(1)^2 \cdot P$				
...	104	$L(1) \cdot L(2) \cdot [L(4) - 1] \cdot P$			
	171	$L(1) \cdot L(2) \cdot [L(5) - L(1)] \cdot P$			

2. Non-graphical factor $P = L(4) - 2L(2) - 1$ (ref. 10 in table 2)

$L(4) - 2L(2) - 1$ is the ACYCLIC polynomial of 


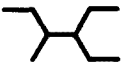
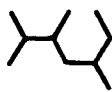
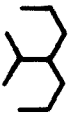
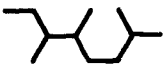
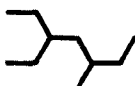
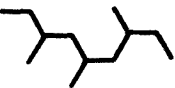
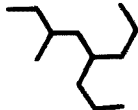
28	$L(1) \cdot L(3) \cdot P$		40	$L(2) \cdot L(3) \cdot P$	
76	$L(1) \cdot L(5) \cdot P$		69	$L(3) \cdot L(3) \cdot P$	
124	$L(1) \cdot L(6) \cdot P$		102	$L(2) \cdot L(5) \cdot P$	
194	$L(1) \cdot L(7) \cdot P$		181/208	$L(3) \cdot L(5) \cdot P$	

Table 10 (continued)

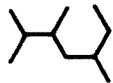
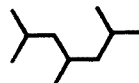
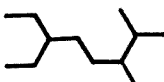
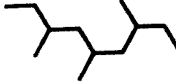

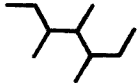
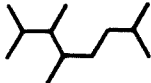
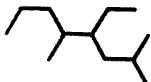





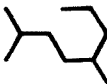
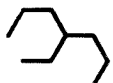
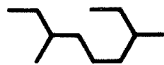
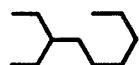

76	$L(2).[L(4) - 1].P$		111	$L(3).[L(4) - 1].P$	
224	$L(2).[L(6) - L(2)].P$		194	$L(3).[L(5) - L(1)].P$	
3. Non-graphical factor $P = L(4) - 2L(2) - 2$ (ref. 9 in table 2)					
$[L(2) - 1].P$ is the ACYCLIC polynomial of 					
79	$L(2).L(4).P$		271	$L(1).L(7).P$	
231	$L(3).L(5).P$				
4. Non-graphical factor $P = L(4) - L(2) - 1$ (reference 13 in table 2)					
P is the ACYCLIC polynomial of 					
9	$L(2).P$				
15	$L(3).P$				
5. Non-graphical factor $P = L(6) - L(4) - L(2) - 1$ (ref. 44 in table 2)					
P is the ACYCLIC polynomial of 					
17	$L(1).P$		59	$[L(4) - 1].P$	
30	$L(3).P$		95	$[L(5) - 1].P$	
89	$L(5).P$				

Table 10 (continued)

6. Non-graphical factor $P = L(4) - L(2)$ (ref. 14 in table 2)

P is the ACYCLIC polynomial of  and unites a more complex group with few patterns





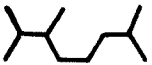
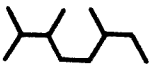
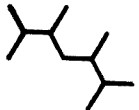
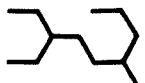
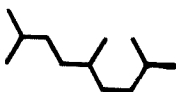
7	$L(5) - L(1)$	$= L(1) \cdot P$	
12	$L(7)$	$= L(3) \cdot P$	
93	$L(11) - 2L(7) + L(3)$	$= [L(7) - 2L(3)] \cdot P$	
95	$L(11) - 2L(7) - 2L(5) + L(3) + 2L(1)$	$= [L(7) - 2L(3) - 2L(1)] \cdot P$	
123	$L(11) - 3L(7) - 2L(5) + L(3) + 2L(1)$	$= L(1)^3 \cdot [L(4) - 3L(2) + 3] \cdot P$	
126	$L(11) - 3L(7) - 3L(5) + L(3) + 3L(1)$	$= L(1) \cdot [L(6) - L(4) - 2L(2) - 1] \cdot P$	
135	$L(11) - 4L(7) - 4L(5) + L(3) + 4L(1)$	$= L(1)^3 \cdot [L(4) - 3L(2) + 2] \cdot P$	
171	$L(12) - 2L(8) - 3L(6) - L(4) + 2L(2) + 1$	$= [L(8) - 2L(4) - 3L(2) - 2] \cdot P$ $= L(1)^2 \cdot L(2) \cdot [L(4) - 3L(2) + 3] \cdot P$	
178	$L(12) - 3L(8) - L(6) + 2L(4) - L(2) - 2$	$= L(1)^2 \cdot [L(6) - 2L(4) + 1] \cdot P$	

Table 10 (continued)

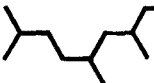
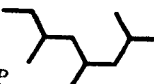
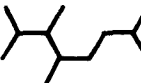
190	$L(12) - 3L(8) - 2L(6) + L(4) - 1$	$= L(1)^2 \cdot [L(6) - 2L(4)] \cdot P$	
194	$L(12) - 3L(8) - 3L(6) + L(2)$	$= [L(8) - 3L(4) - 3L(2) - 1] \cdot P$ $= L(1) \cdot L(3) \cdot [L(4) - 2L(2) - 1] \cdot P$ $= L(1)^2 \cdot [L(2) - 1] \cdot [L(4) - 2L(2) - 1] \cdot P$	
271	$L(12) - 4L(8) - 4L(6) + L(2)$	$= L(1)^2 \cdot [L(2) - 1] \cdot [L(4) - 2L(2) - 2] \cdot P$	


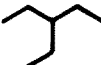

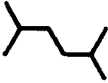
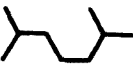
Table 11

Some trees which have cyclic factors

These are simple illustrative examples; they do not form an exhaustive list. This type of factorisation is of particular interest in that it represents the only kind discovered so far that yields factors that are all capable of a graphical representation. In this table, $R(n)$ denotes the characteristic polynomial of a cycle, i.e.

$$L(n) - L(n - 2) - (-1)^n \cdot 2$$

Refs. are to table 1:

11	$L(6) - 2L(2) - 1$	$= R(4) \cdot L(2)$	
13	$L(7) - L(3) - 2L(1)$	$= R(6) \cdot L(1)$	
16	$L(7) - 2L(3)$	$= R(4) \cdot L(3)$	
23	$L(8) - 2L(4) + 1$	$= R(4) \cdot L(4)$	
35	$L(9) - 2L(5) + L(1)$	$= R(4) \cdot L(5)$	

3.5. THE RELATIONSHIP BETWEEN TREES AND RING-CONTAINING STRUCTURES

In the previous section, the occurrence of non-graphical factors common to both trees and ring-containing structures was commented on. It is well known that tree factors occur too. Perhaps the simplest example is that of an annulene. A $2n + 2$ membered ring contains $L(n)$ as a factor [2,44], and this is only one example of many [2].

The converse situation, where a ring is a factor of a tree, also happens, but seems to have been less remarked upon. Table 11 shows a few examples of this, and the subject of factoring ring-containing structures, and of factoring trees in terms of ring-containing structures, is under more extensive investigation. The examples of table 11 are of particular interest because, unlike the factorisations obtained by the systematic extraction of trees reported here, factorisation in terms of rings seems often to yield factors which are all graphical. The implication of this, that certain cyclic graphs also can be expressed as a ratio of trees, is difficult to relate to a visual concept.

Appendix

Several of the lists shown or referred to are also available in computer-readable form from the author's institution at a small charge for costs. These are the structure codes and characteristic polynomials (table 1); N -tuple codes of table 1 (not shown); lists of non-graphical polynomials (table 2), and the factorisation references shown in table 3. A standard 128 byte length record is used for each entry, on a 5.25 inch diskette in IBM-PC format.

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