

REVIEW

THE CHARACTERISTIC POLYNOMIAL OF A CHEMICAL GRAPH^{★, ☆}Nenad TRINAJSTIĆ[†]*Department of Marine Sciences, Texas A&M University, Galveston, Texas 77553, USA*

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"The calculation of characteristic polynomials of graphs of any size is usually extremely tedious, . . ."

Harary, King, Mowshowitz and Read [1].

Abstract

We list uses of, and the computational methods for the characteristic polynomial of a (chemical) graph. Four computational methods are singled out for more detailed presentation. These are the graphical methods of Sachs, the recurrence formulae for several classes of simple graphs, the method based on Ulam subgraphs, and the Le Verrier–Faddeev–Frame recursive method. The latter method appears, at present, to be the most efficient procedure for the computation of the characteristic polynomials of graphs of sizes with up to even a few hundred sites.

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1. Introduction

The characteristic or spectral polynomial $P(G; x)$ of a (chemical) graph G is the characteristic polynomial of its adjacency matrix [2]:

$$P(G; x) = \det |xI - A| = 0, \quad (1.1)$$

where A and I are, respectively, the adjacency matrix of a graph G with N vertices and the $N \times N$ unit matrix. A graph eigenvalue x_i is a zero of the characteristic polynomial:

$$P(G; x_i) = 0 \quad (1.2)$$

for $i = 1$ to N . The complete set of graph eigenvalues x_1, x_2, \dots, x_N forms the spectrum of the graph [3]. The eigenvalues are real and the interval in which the graph eigenvalues lie is bounded. According to Frobenius' theorem [4], the limits of the graph spectrum are determined by the maximal valency of a vertex $d(\max)$ in G :

$$-d(\max) \leq x_i \leq d(\max). \quad (1.3)$$

Among connected graphs, equality is achieved on the right-hand side iff all vertices have the same degree, while equality is achieved on the left-hand side iff also the graph is bipartite; in either case, these maximally extreme eigenvalues are non-degenerate.

The characteristic polynomial of a graph is most often given in the coefficient form:

$$P(G; x) = \sum_{n=0}^N a_n x^{N-n}. \quad (1.4)$$

The coefficients a_0, a_1, \dots, a_N are graph invariants and are related to the structure of a graph in a simple way [2-6].

The characteristic polynomial can also be given in terms of its zeros [7]:

$$P(G; x) = \prod_{i=1}^N (x - x_i). \quad (1.5)$$

If the permanent of the adjacency matrix is introduced instead of the determinant in (1.1), the permanent polynomial $\mathcal{P}(G; x)$ of G is obtained [8]:

$$\mathcal{P}(G; x) = \text{per } |xI - A| = 0. \quad (1.6)$$

The characteristic polynomial is an important structural invariant, although it is not always unique to a single graph because of the fact that non-isomorphic

graphs may possess identical characteristic polynomials [9–17]. Non-isomorphic graphs with identical spectra are called isospectral or cospectral graphs [1,3,9,14,18,19]. A special class of isospectral graphs is named endospectral graphs [16,20].

2. The uses of the characteristic polynomial

The characteristic polynomial of a graph continues to hold current chemical interest because it arises in numerous applications [20–25]. Some of these applications will be briefly summarized below:

(i) The characteristic polynomial (and the related acyclic (reference, matching) polynomial [26–29]) is used in the topological theory of aromaticity [21,30–33].

(ii) The characteristic polynomial is useful in predicting the relative stabilities of conjugated hydrocarbons [34] and in the formulation of the topological effect on molecular orbitals (TMO) concept [35,36].

(iii) The last two coefficients (a_{N-2} and a_N) in the characteristic polynomials of benzenoids, arenecyclobutadienoids (such as benzocyclobutadienoids), azulenoids, pentalenoids, etc. can be used for counting Kekulé valence structures and Dewar valence structures [37–39]; quantities that represent the basis of resonance-theoretical approaches such as the structure-resonance theory [40–42] and the conjugated-circuit model [43–46].

(iv) The characteristic polynomial has found application in quantum chemistry [22,23,47–50], chemical kinetics [51], dynamics of oscillatory reactions [52], solutions of Navier–Stokes equations [53] and in statistical mechanics because it serves as a generating function for dimer statistics on trees such as Bethe lattices [54].

(v) The coefficients of the characteristic polynomial may be interpreted as the counts of random walks over the structural network [55–57]. Random walks on the structural networks (lattices) are fundamental in several areas in representing the path of a diffusing particle or in modelling the conformations of flexible macromolecules, especially in dilute solution [58–61].

(vi) The characteristic polynomials are related to several other graph invariants such as spectral moments [55,56,62]. They are also auxiliary functions for counting subgraphs of various kinds belonging to a given (chemical) graph [2–6,21,29,37,48,63–65].

(vii) The characteristic polynomial can be used for a partial ordering of forests [66].

(viii) The characteristic polynomial can be used for counting the spanning trees of labelled planar graphs [67,68].

(ix) The characteristic polynomial can be used in analysis of NMR spectra [69].

(x) The characteristic polynomials may be used for coding (chemical) graphs [70].

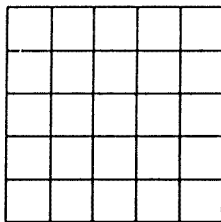
(xi) The characteristic polynomials may arise in the *Y*-conjugation model of cyanine dyes (which are depicted by polymethine graphs) [71].

(xii) The characteristic polynomial serves as the generator for the characteristic equations of a graph [20]. (The characteristic equations for a graph are defined as the system of equations for the coefficients of the characteristic polynomial.)

(xiii) The characteristic polynomial has also been found useful in areas other than mathematics [1–3,5,9,20,27,72–75], physics [53,54,58–61] and chemistry. For example, in computer science (e.g. [76]) and biology (e.g. [77]).

3. Computational methods for the characteristic polynomial

The computation of the characteristic polynomial is rather involved due to the combinatorial complexity of the problem [1]. To illustrate this point, let us consider a planar square lattice graph with 36 vertices *I*



I

The characteristic polynomials of this graph, which is not a particularly complex structure, is given by [78]:

$$\begin{aligned}
 P(I; x) = & x^{36} - 60x^{34} + 1572x^{32} - 23,772x^{30} + 231,126x^{28} \\
 & - 1,523,844x^{26} + 7,005,754x^{24} - 22,757,380x^{22} \\
 & + 52,393,405x^{20} - 85,052,332x^{18} + 96,104,022x^{16} \\
 & - 73,969,028x^{14} + 37,486,225x^{12} - 11,814,292x^{10} \\
 & + 2,074,464x^8 - 153,664x^6.
 \end{aligned} \tag{3.1}$$

The largest coefficient (i.e. the coefficient of x^{16}) is of the order of 96 million, which indicates the combinatorial complexity involved in the computation of the characteristic polynomial.

There are many methods available for the computation of the characteristic polynomials for graphs. Some of them are summarized below:

(i) The Laplace expansion of the determinant (1.1), which is unwieldy for larger systems.

(ii) The matrix diagonalization procedure and the use of the Viète formula (1.5). There are a number of methods available for the diagonalization of a (adjacency) matrix [79]: Jacobi's method, Givens' method, the QR-algorithm, and many others.

(iii) Direct graphical constructions such as Sachs' procedure [5] have been explored rather extensively for chemical graphs [3,4,19,21,29,37,48,80–90]. Early graphical procedures resulted from the need to carry out simple MO calculations in spite of the lack of computers. Amongst the first to propose the construction of the characteristic polynomial by breaking a graph into smaller transferable fragments for which the characteristic polynomials can be easily computed were Samuel [91], Coulson [4], and Heilbronner [92]. Graphical constructions have shown a great conceptual value, but have a practical difficulty in the form of an enormous increase of combinatorial possibilities of basic figures with the increase of the size of the (chemical) graph. This problem cannot be avoided even if the graphical construction is carried out by computer [93–95].

(iv) The characteristic polynomials of classes of simple graphs (molecules) such as chains (polyenes) and cycles (annulenes) can be obtained by recurrence formulae [1,3,21,92,96].

(v) Special methods such as the transfer matrix method [97,98], the partition technique [99–101], the polynomial matrix method [102–105], the pruning technique [106–109], the ultimate pruning technique [110], the symmetry blocking method [111,112], the operator technique [113], the Chebishev expansion [56,114–116], the use of the Frobenius matrix [117], the use of power sum symmetric functions [118,119], the use of symmetry properties of a structure [120], the use of powers of the adjacency matrix [121], the use of the Ulam subgraphs [122,123], the use of a functional group-like concept [124–126], etc.

(vi) Recursive techniques such as those of Le Verrier [127,128], Faddeev [129] and Frame [130].

There are too many methods in the above to be reviewed in this single article. Here, we will present briefly the method of Sachs, the recurrence formulae for simple graphs, the method based on the Ulam subgraphs, and the recursive techniques of Le Verrier, Faddeev, and Frame.

4. The method of Sachs for computing the characteristic polynomial

The method of Sachs [5] relates the structure of a graph G and the coefficients of its characteristic polynomial. All coefficients of $P(G; x)$ may be obtained from the Sachs formula [37]:

$$a_n = \sum_{s \in \mathcal{S}_n} (-1)^{p(s)} 2^{c(s)}, \quad (4.1)$$

where s is a Sachs graph, \mathcal{S}_n a set of all Sachs graphs with n vertices, while $p(s)$ and $c(s)$ denote, respectively, the total number of components and the total number of cyclic components in s . The components of a Sachs graph can be either complete graphs K_2 or cycles C_m . Then, if α_m is the number of such m -site components, $\sum_m m \alpha_m = n$.

The characteristic polynomial can now be expressed in the following form by introducing (4.1) into (1.4):

$$P(G; x) = \sum_{n=0}^N \sum_{s \in \mathcal{S}_n} (-1)^{p(s)} 2^{c(s)} x^{n-N}. \quad (4.2)$$

If the cyclic components are neglected, the characteristic polynomial reduces to the acyclic polynomial of a graph [30–32]:

$$P^{ac}(G; x) = \sum_{n=0}^N \sum'_{s \in \mathcal{S}_n} (-1)^{p(s)} x^{n-N}. \quad (4.3)$$

The two polynomials are, of course, identical only for acyclic graphs [32]. The characteristic polynomial and acyclic polynomial are basic quantities in a topological (graph-theoretical) resonance energy model [21, 30–33, 48, 65].

The Sachs formula was also adopted for computing coefficients of the characteristic polynomial of a vertex-weighted and edge-weighted graph G_{vew} [21, 80, 131–133]:

$$a_n = \sum_{s \in \mathcal{S}_n} (-1)^{p(s)} 2^{c(s)} \prod_i^s h_i \prod_j^{K_2 \text{ in } s} k_j \prod_{j'}^{C \text{ in } s} k_{j'}. \quad (4.4)$$

In the above equation, symbols have the following meaning: h_i is the weight of the i th vertex depicted by a loop, the first product gives the contribution from all the weighted vertices i with weights h_i in s , k_j is the weight of the j th edge, which may be either a K_2 -component of s or an edge in a C -component of s , the second product

5. The characteristic polynomials of some classes of chemical graphs

Graphical constructions of the characteristic polynomial lead to the recurrence formulae for some classes of simple (chemical) graphs. Several of these will be shown below.

(i) Chains

Chains may be used to depict the carbon skeleton of n -alkanes or the π -skeleton of linear polyenes. We denote the characteristic polynomials of chains with n vertices by L_n for simplicity. The recurrence formula for the characteristic polynomials of chains is given by [92]:

$$L_n = x L_{n-1} - L_{n-2}, \quad (5.1)$$

with $L_0 = 1$ and $L_1 = x$.

The tables of the characteristic polynomials for chains with up to $n = 20$ are given elsewhere [21,80].

(ii) Trees

Trees may be used to depict acyclic structures such as branched alkanes. The generating formula for the characteristic polynomial T_n of a tree with n vertices is as follows [1,21,92,134]:

$$T_n = T_{n-e} - T_{n-(e)}, \quad (5.2)$$

where T_{n-e} and $T_{n-(e)}$ are the characteristic polynomials of subgraphs obtained after deleting from the tree, respectively, the edge e , and the edge e along with its incident vertices. As an example, we apply the above formula to the tree \mathcal{J} in table 2.

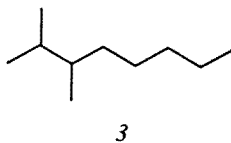
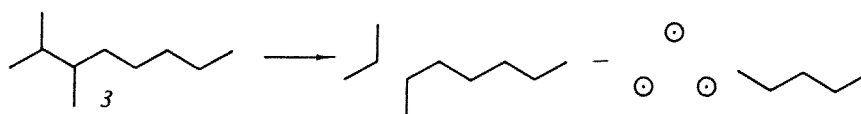


Table 2

The computation of the characteristic polynomial
for the tree \mathcal{J} by formula (5.2)



$$T_{10} = L_3 \cdot L_7 - L_1^3 \cdot L_5 = x^{10} - 8x^8 + 26x^6 - 27x^4 + 8x^2$$

The strategy of using (5.2) is to break up the tree into constituting chains in the smallest possible number of steps. Note that the chain is the unbranched tree.

For large and highly branched trees, the application of (5.2) becomes rather complicated. In that case, the pruning technique of Balasubramanian and Randić [106–110] is recommended.

(iii) Cycles

Cycles C_n ($n \geq 3$) may be used to depict the carbon skeleton of cyclo-alkanes or the π -skeleton of annulenes. The generating formula for the characteristic polynomial of a cycle with n vertices is given by [1,21,92,134]:

$$P(C_n; x) = L_n - L_{n-2} - 2. \quad (5.3)$$

The idea behind this formula is to reduce the cycle C_n into constituting chains in two steps: The first step is to remove an edge from C_n and the second step is to remove this edge, incident vertices and adjacent edges from C_n . In the first case we obtain a chain with n vertices whose characteristic polynomial is L_n , and in the second case we obtain a chain with $n - 2$ vertices whose characteristic polynomial is L_{n-2} . The term -2 is the contribution for cycle closure.

(iv) Möbius cycles

Möbius cycles C_n^* ($n \geq 3$) are cycles with at least one edge (or more generally, an odd number of edges) with the weight -1 [135,136]. They may be used to describe Möbius annulenes [137–139]. The generating formula for the characteristic polynomial of a Möbius cycle with n vertices is again based on the two-step reduction procedure, which by the removal of the edge e (the first step) and by the removal of the edge e , incident vertices and adjacent edges (the second step) from C_n^* produces two chains: a chain with n vertices whose characteristic polynomial is L_n and a chain with $n - 2$ vertices whose characteristic polynomial is L_{n-2} . The generating formula for the characteristic polynomials of Möbius cycles is then given by:

$$P(C_n^*; x) = L_n - L_{n-2} + 2. \quad (5.4)$$

The term $+2$ is the contribution for the Möbius cycle closure.

6. The characteristic polynomial and Ulam subgraphs of a graph

Ulam subgraphs of a graph G represent a collection of subgraphs $G - v_i$ obtained by the consecutive removal of a single vertex v_i ($i = 1, 2, \dots, N$) from G until the vertex-set $\{v_i\}$ of G is exhausted [123]. The sum of the characteristic poly-

Table 3
 Characteristic polynomials for the collection of Ulam subgraphs belonging to the weighted graph 2

Weighted graph 2	Ulam subgraph $2 - v_i$	Characteristic polynomial $P(2 - v_i; x)$
		$x^4 - 3x^2 + 1$
		$x^4 - hx^3 - (k^2 + 2)x^2 + 2hx + k^2$
		$x^4 - hx^3 - (2k^2 + 1)x^2 + hx + k^2$
		$x^4 - hx^3 - (2k^2 + 1)x^2 + hx + k^2$
		$x^4 - hx^3 - (k^2 + 2) + 2hx + k^2$
$\sum_i P(2 - v_i; x) = 5x^4 - 4hx^3 - 3(2k^2 + 3)x^2 + 6hx + (4k^2 + 1)$		

nomials $P(G - v_i; x)$ of Ulam subgraphs $G - v_i$ ($i = 1, 2, \dots, N$) of G is equal to the derivative of the characteristic polynomial $P'(G; x)$ of G :

$$P'(G; x) = \sum_i P(G - v_i; x). \quad (6.1)$$

The characteristic polynomial of G is then given by:

$$P(G; x) = \int P'(G; x) dx, \quad (6.2)$$

where the integration constant is equal to the negative determinant of the adjacency matrix of G .

As an example, we consider the weighted graph 2. The corresponding Ulam subgraphs and their polynomials are given in table 3. If we integrate $P'(2; x)$ and evaluate the integration constant ϵ :

$$\epsilon = -\det |A| = -(2k^2 + h), \quad (6.3)$$

the characteristic polynomial of 2 is obtained.

7. The Le Verrier–Faddeev–Frame method for computing the characteristic polynomial

The very efficient method for the computation of the characteristic polynomial for any (chemical) graph is the recursive approach of Le Verrier, Faddeev, and Frame [127–130]. This approach was introduced by Le Verrier in 1840, and was used in the perturbative computation of the orbits of planets in our solar system. The approaches developed by Faddeev and by Frame essentially reduce to Le Verrier's method [140]. Faddeev's approach is a modification, while Frame introduced a novel algebraic style. The Le Verrier–Faddeev–Frame method has been shown by Balasubramanian [22, 24, 57, 78, 141–143] and by the Zagreb Group [144] to be a computationally convenient procedure for generating the characteristic polynomials for large chemical graphs.

Recently, Barakat [118] has also analyzed the Frame method and has shown that it is based on symmetric functions and the Newton identities.

The recursive formulae for computing the coefficients a_n of the characteristic polynomial of G , given in the following form:

$$\begin{aligned} P(G; x) = \det |xI - A| &= x^N - a_1 x^{N-1} - a_2 x^{N-2} - \dots \\ &\dots - a_{N-1} x - a_N = 0, \end{aligned} \quad (7.1)$$

are presented below for each of the three procedures.

(i) *Le Verrier's procedure*

$$a_n = (1/n)(\text{tr } A^n - a_1 \text{tr } A^{n-1} - \dots - a_{n-1} \text{tr } A), \quad (7.2)$$

where $\text{tr } A$ is the trace of the matrix A .

(ii) *Faddeev's procedure*

$$a_n = (1/n) \text{tr } A_n. \quad (7.3)$$

(iii) *Frame's procedure*

$$a_n = (1/n) \text{tr } A B_{n-1}. \quad (7.4)$$

Equations (7.2) and (7.3) are related by:

$$A_n = A^n - a_1 A^{n-1} - \dots - a_{n-1} A, \quad (7.5)$$

and eqs. (7.3) and (7.4) by:

$$A_n = A B_{n-1}, \quad (7.6)$$

where B_{n-1} are $N \times N$ matrices which can be obtained from the recursive relationship:

$$B_{n-1} = A_{n-1} - a_{n-1} I. \quad (7.7)$$

Note that:

$$B_N = A_N - a_N I = \mathbf{0}. \quad (7.8)$$

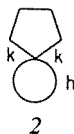
Since eqs. (7.2)–(7.4) can be easily transformed among themselves, all three of the above procedures reduce to the same method for computing the characteristic polynomial of a graph.

The algorithm for computing the coefficients of the characteristic polynomial for a given (chemical) graph by the Le Verrier–Faddeev–Frame method can be organized as follows:

$$\begin{aligned} G \rightarrow A = A_1 \rightarrow a_1 \rightarrow B_1 \rightarrow A_2 \rightarrow a_2 \rightarrow \dots \\ \dots \rightarrow a_{N-1} \rightarrow B_{N-1} \rightarrow A_N \rightarrow a_N \rightarrow B_N = \mathbf{0}. \end{aligned} \quad (7.9)$$

Table 4

The computation of the characteristic polynomial for the weighted graph 2 by the Le Verrier – Faddeev – Frame method



(I) $a_0 = 1$ (by definition)

$$A = \begin{bmatrix} h & k & 0 & 0 & k \\ k & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ k & 0 & 0 & 1 & 0 \end{bmatrix} = A_1$$

(II) $a_1 = \text{tr } A_1 = h$

$$B_1 = A_1 - a_1 I = \begin{bmatrix} 0 & k & 0 & 0 & k \\ k & -h & 1 & 0 & 0 \\ 0 & 1 & -h & 1 & 0 \\ 0 & 0 & 1 & -h & 1 \\ k & 0 & 0 & 1 & -h \end{bmatrix}$$

$$A_2 = AB_1 = \begin{bmatrix} 2k^2 & 0 & k & k & 0 \\ 0 & k^2 + 1 & -h & 1 & k^2 \\ k & -h & 2 & -h & 1 \\ k & 1 & -h & 2 & -h \\ 0 & k^2 & 1 & -h & k^2 + 1 \end{bmatrix}$$

(III) $a_2 = (1/2) \text{tr } A_2 = 2k_2 + 3$

$$B_2 = A_2 - a_2 I = \begin{bmatrix} -3 & 0 & k & k & 0 \\ 0 & -(k^2 + 2) & -h & 1 & k^2 \\ k & -h & -(2k^2 + 1) & -h & 1 \\ k & 1 & -h & -(2k^2 + 1) & -h \\ 0 & k^2 & 1 & -h & -(k^2 + 2) \end{bmatrix}$$

$$A_3 = AB_2 = \begin{bmatrix} -3h & -2k & k & k & -2k \\ -2k & -h & -(k^2 + 1) & k^2 - h & 1 \\ k & -(k^2 + 1) & -2h & -2k^2 & k^2 - h \\ k & k^2 - h & -2k^2 & -2h & -(k^2 + 1) \\ -2k & 1 & k^2 - h & -(k^2 + 1) & -h \end{bmatrix}$$

Table 4 (continued)

$$(IV) a_3 = (1/3) \operatorname{tr} A_3 = -3h$$

$$B_3 = A_3 - a_3 I = \begin{bmatrix} 0 & -2k & k & k & -2k \\ -2k & 2h & -(k^2+1) & k^2-h & 1 \\ k & -(k^2+1) & h & -2k^2 & k^2-h \\ k & k^2-h & -2k^2 & h & -(k^2+1) \\ -2k & 1 & k^2-h & -(k^2+1) & 2h \end{bmatrix}$$

$$A_4 = AB_3 = \begin{bmatrix} -4k^2 & k & -k & -k & k \\ k & -(3k^2+1) & k^2+h & -k^2 & -(k^2+h) \\ -k & k^2+h & -(3k^2+1) & k^2 & -k^2 \\ -k & -k^2 & k^2 & -(3k^2+1) & k^2+h \\ k & -(k^2+h) & -k & k^2+h & -(3k^2+1) \end{bmatrix}$$

$$(V) a_4 = (1/4) \operatorname{tr} A_4 = -(4k^2+1)$$

$$B_4 = A_4 - a_4 I = \begin{bmatrix} 1 & k & -k & -k & k \\ k & k^2 & k^2+h & -k^2 & -(k^2+h) \\ -k & k^2+h & k^2 & k^2 & -k^2 \\ -k & -k^2 & k^2 & k^2 & k^2+h \\ k & -(k^2+h) & -k^2 & k^2+h & k^2 \end{bmatrix}$$

$$A_5 = AB_4 = \begin{bmatrix} 2k^2+h & 0 & 0 & 0 & 0 \\ 0 & 2k^2+h & 0 & 0 & 0 \\ 0 & 0 & 2k^2+h & 0 & 0 \\ 0 & 0 & 0 & 2k^2+h & 0 \\ 0 & 0 & 0 & 0 & 2k^2+h \end{bmatrix}$$

$$(VI) a_5 = (1/5) \operatorname{tr} A_5 = 2k^2+h$$

$$B_5 = A_5 - a_5 I = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} = 0$$

$$P(2; x) = x^5 - hx^4 - (2k^2+3)x^3 + 3hx^2 + (4k^2+1)x - (2k^2+h)$$

Computer programs have been developed based on this algorithm [141,142]. An example of computing the characteristic polynomial by the above algorithm is given for the weighted graph 2 in table 4.

The efficiency of the Le Verrier–Faddeev–Frame method can be seen from the computation time needed to generate the characteristic polynomial of I , which was 12 seconds on VAX11/730 [78].

8. Conclusions

In 1972, two papers appeared in *Theoretica Chimica Acta* (the first by Hosoya [63] and the second by the Zagreb Group [37]) reporting two independent graphical methods for computing the characteristic polynomial of chemical graphs. In 1977, the present author published a fairly detailed review in *Croatica Chemica Acta* on the graphical computation of the characteristic polynomial of a conjugated system using the Sachs formula [80]. Soon after this publication appeared, it became clear that the Sachs method, although very instructive and elegant, is not computationally practical. This fact inspired the search for efficient computational methods for the characteristic polynomial of a chemical graph. Persistent in this objective were Hosoya, Balasubramanian, Randić, Dias, and the Zagreb Group. The most efficient method to date appears to be the procedure of Le Verrier, Faddeev and Frame, which was uncovered independently by Balasubramanian and by the Zagreb Group. This method provides an excellent algorithm for the computer generation of the characteristic polynomials for graphs of chemical interest. Thus, we are in a position similar to that of eleven years ago. At that time we had the Sachs procedure and thought how elegant and efficient the method was. However, very soon we found through, for example, the use of the topological resonance energy model that we needed a much more efficient computational procedure if we wished to consider large systems. Now, we have the "old" and elegant Le Verrier–Faddeev–Frame method, recently rediscovered and adopted for use on the computer for large graphs; it appears to be so efficient that it may well remain in use for many years.

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