

# Computer Generation of Characteristic Polynomials of Edge-Weighted Graphs, Heterographs, and Directed Graphs

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The computer code developed previously (K. Balasubramanian, *J. Computational Chem.*, **5**, 387 (1984)) for the characteristic polynomials of ordinary (nonweighted) graphs is extended in this investigation to edge-weighted graphs, heterographs (vertex-weighted), graphs with loops, directed graphs, and signed graphs. This extension leads to a number of important applications of this code to several areas such as chemical kinetics, statistical mechanics, quantum chemistry of polymers, and unsaturated systems containing heteroatoms which include bond alternation. The characteristic polynomials of several edge-weighted graphs which may represent conjugated systems with bond alternations, heterographs (molecules with heteroatoms), directed graphs (chemical reaction network), and signed graphs and lattices are obtained for the first time.

## I. INTRODUCTION

The evaluation of the characteristic polynomials of graphs has been the subject of numerous investigations<sup>1-36</sup> in recent years. The evaluation of these polynomials for graphs is generally regarded as a tedious problem owing to the combinatorial complexity involved in this problem. There are a number of chemical applications of these polynomials, many of which are discussed in the literature,<sup>1-34</sup> particularly the more recent references.<sup>10-13</sup>

In summary, the characteristic polynomials have applications in chemical kinetics,<sup>37</sup> quantum chemistry, dynamics of oscillatory reactions, and in determining the stabilities of reaction networks,<sup>35</sup> lattice statistics,<sup>38</sup> estimating the stabilities of conjugated systems,<sup>27</sup> formulation of TEMO theorem,<sup>39</sup> enumeration of walks and self-returning walks,<sup>3</sup> and electronic structure of organic polymers and periodic structures.<sup>4,11</sup>

In earlier investigations, we discussed an algorithm<sup>2</sup> and computer code<sup>1</sup> to generate the characteristic polynomials of graphs containing a large number of vertices with very little computer time using an elegant recur-

sive matrix product method. This method was also shown to be applicable to characteristic polynomials of organic polymers and periodic structure.<sup>4</sup> The characteristic polynomials of many graphs and lattices containing a large number of vertices could be obtained for the first time using that computer code.<sup>1</sup>

The present investigation is aimed at developing a computer code to evaluate the characteristic polynomials of edge-weighted graphs, vertex-weighted graphs, and directed graphs. We extend our earlier code to calculate the characteristic polynomials of edge-weighted and vertex-weighted graphs. We develop a modified code to calculate the characteristic polynomials of directed graphs. Section II describes the method of investigation while Section III reports results and discussions.

## II. METHOD OF CALCULATING CHARACTERISTIC POLYNOMIALS OF WEIGHTED AND DIRECTED GRAPHS.

The adjacency matrix of an edge-weighted graph,  $A$ , is defined as

$$A = \begin{cases} 0 & \text{if } i = j \\ w_{ij} & \text{if } i \neq j \text{ and if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases} \quad (1)$$

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where  $w_{ij}$  is the weight of the edge connecting the vertices  $i$  and  $j$ . The normal adjacency matrix of a graph differs from the above matrix in that the weights of all the edges are the same and set to unity in the adjacency matrix of an ordinary graph. The adjacency matrix of a vertex-weighted graph is defined as

$$A = \begin{cases} v_i & \text{if } i = j \\ 1 & \text{if } i \neq j \text{ and if } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases} \quad (2)$$

where  $v_i$  is the weight of the vertex  $i$ . Note that for some vertices,  $v_i$  could be zero. There is also the third possibility in which both vertices and edges could be weighted with different weights.

$$A = \begin{cases} v_i & \text{if } i = j \\ w_{ij} & \text{if } i \neq j \text{ and } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases} \quad (3)$$

The edge-weighted graphs occur in a number of applications. If one interprets the weights as the rate constants and the vertices as the chemical species participating in a chemical reaction, then the associated adjacency matrix is the matrix of rate constants. One of the ramifications of Hückel theory or extended Hückel theory is to remove the constraint that all the nearest neighbors interact the same way. A popular method called "bond alternation" is to allow different weights for single and double bonds. Then the associated graph and its adjacency matrix would be weighted. In statistical mechanics, one has to deal with nonisotropic lattices. The associated lattice graph would then be weighted. Quantum chemical problems dealing with organic molecules containing heteroatoms lead to vertex- and edge-weighted graphs. The heteroatom node is sometimes denoted by a graph which contains loops at that node. Thus edge/vertex weights appear in many applications.

The characteristic (spectral) polynomial of a weighted graph is defined as the secular determinant of the associated weighted adjacency matrix shown below

$$P_G(\lambda) = |A - \lambda I| \quad (4)$$

In earlier papers<sup>1,2</sup> we showed the power of a

method which we call Frame's method and later called Leverrier-Faddeev method by Krivka *et al.*<sup>28</sup> (also see ref. 16) for evaluating the characteristic polynomial of an ordinary graph. This method reduces a numerically complex problem of determinant expansion to a simple recursive matrix product algorithm. The method runs as follows. If one constructs, the matrix  $B_k$ 's as follows recursively, the coefficients of the characteristic polynomials are generated as the traces of  $B_k$ 's.

$$C_1 = \text{Trace } A \quad (5)$$

$$B_1 = A(A - C_1 I), \quad (6)$$

$$C_2 = \frac{1}{2} \text{Trace } B_1, \quad (7)$$

$$B_2 = A(B_1 - C_2 I) \quad (8)$$

⋮

$$B_{n-1} = A(B_{n-2} - C_{n-1} I) \quad (9)$$

$$C_n = \left(\frac{1}{n}\right) \text{Trace } B_{n-1} \quad (10)$$

The characteristic polynomial of the matrix  $A$  is then given by (11)

$$P_G(\lambda) = \lambda^n - C_1 \lambda^{n-1} - C_2 \lambda^{n-2} \dots - C_{n-1} \lambda - C_n \quad (11)$$

The above algorithm is valid for any matrix, although, in our earlier code<sup>1</sup> we assumed the matrix is the adjacency matrix of the graph. Thus the structure of the code developed earlier takes advantage of the fact that the matrix is real symmetric and the off-diagonal elements of the connected vertices are all equal to 1. Consequently, the code developed up to now could be used only for ordinary graphs. In this investigation we extend the code in many ways which enables computations of the polynomial of any weighted graph.

We develop two computer programs in Fortran 77, one for edge/vertex-weighted graphs but not directed, so the adjacency matrix is still real symmetric. In this case many parts of the earlier code are modified to take into account the fact that the weights are different. In fact, the weights have to be read in for this code for the various edges and vertices. The other code is for directed graphs which we consider later. Since the weights of the edges could be non-integral numbers, the integer arithmetic

used in the earlier code does not work. The code was modified to double precision real arithmetic.

The input description for the computer code to evaluate the characteristic polynomials of edge/vertex weighted graphs is shown in Table I. Table II shows a sample input for which the output is shown in Table III. A copy of this computer code or the code for directed graphs could be obtained from the author.

A directed graph is a graph in which the edges have direction. Thus arrows are added to the edges pointing the direction of flow (from vertex  $i$  to  $j$  or  $j$  to  $i$ ). Also, a directed graph could be edge/vertex weighted. In general, the edge from  $i$  to  $j$  need not have the same weight as an edge from  $j$  to  $i$ . This is the case in chemical kinetics, since the rate constant for the forward reaction is not the same as the rate constant for the reverse reaction.

The adjacency matrix of a directed graph is thus nonsymmetric. This leads to a problem in that our earlier code takes advantage of symmetric nature of the matrix in storage as well as computation. Thus, for this case a simple modification of the code would not be enough. We rewrote the entire code which stores the whole matrix in a two-dimensional array rather than the upper triangle

**Table II.** Sample input for the weighted  $L_6$  graph (linear chain of length 6) with bond alteration. The weights of alternate bonds are 1.159 or 1.0.

Card		
1	1	
2	weighted $L_6$ ( $w_1/w_2 = 1.159$ )	
3	6	
4		
5	1	1
6	1.159	
7	1	2
8	1.0	
9	1	3
10	1.159	
11	1	4
12	1.0	
13	1	5
14	1.159	

in a one-dimensional array. Further, the input for this code is different since the weights of edges  $i \rightarrow j$  and  $j \rightarrow i$  could be different and therefore must be read in. Table IV shows the input description for the characteristic polynomials of directed graphs. Note that the difference between this input and the earlier input is that all the neighbors of a given vertex (not just the ones with labels less than the given vertex) and the weights of the corresponding edges must be read in.

A class of graphs called signed graphs and Mobius graphs fall in the general category

**Table I.** Input description for the program to compute the characteristic polynomials of edge/vertex weighted graphs.

Card	Format	Input Variable	Description
1	16I5	NGRAPH	Number of graphs to be processed
		For each graph read the following cards	
2	10A8	TITLE	Name of the graph
3	16I5	N, NWT	N: Number of vertices in the graph NWT = 1 if the graph is edge or vertex weighted, 0 otherwise
		For each vertex read the following cards	
4	16I5	M,  (ID(I), I = 1,M)	Number of neighbors of this vertex with labels less than the label of the vertex  The labels of the M vertices which are neighbors of this vertex with smaller labels (If M = 0 leave this blank)
		if NWT = 1 and M $\neq$ 0 read the following card	
5	8F10.5	(W(I), I = 1,M),HET	W(I) = weights of the corresponding edges HET: weight of this vertex. Set to zero if this vertex is not a heteroatom or does not carry loops.

**Table III.** Sample output for the input in Table II.

WEIGHTED L6 (W1/W2 = 1.159)																			
VERTEX	2NEIGHBORS WITH LABELS LESS THAN											THIS VERTEX	1						
1.15900	0.00000																		
VERTEX	3NEIGHBORS WITH LABELS LESS THAN											THIS VERTEX	2						
1.00000	0.00000																		
VERTEX	4NEIGHBORS WITH LABELS LESS THAN											THIS VERTEX	3						
1.15900	0.00000																		
VERTEX	5NEIGHBORS WITH LABELS LESS THAN											THIS VERTEX	4						
1.00000	0.00000																		
VERTEX	6NEIGHBORS WITH LABELS LESS THAN											THIS VERTEX	5						
1.15900	0.00000																		
LOWER TRIANGLE OF THE ADJ MATRIX OF THE GRAPH																			
0.00	1.16	0.00	0.00	1.00	0.00	0.00	0.00	0.00	1.16	0.00	0.00	0.00	0.00	1.00	0.00	0.00			
0.00	0.00	0.00	1.16	0.00															
COEFS IN CHARPOLY																			
				1.0000					0.0000					-6.0298					0.0000
				9.0998					0.0000					-2.4238					

**Table IV.** Input description for the characteristic polynomials of directed graphs. Cards 1-3 same as Table II.

Card	Format	For each vertex read the following cards	
		Input Variable	Description
4	16I5	M (ID(I), I = 1,M)	Number of all neighbors of this vertex The labels of all the neighbors of this vertex if M ≠ 0 and NWT = 1 read
5	8F10.6	(W(I), I = 1,M), HET	W(I) = weight of the edge from I to ID(I) HET: weight of the vertex

of directed graphs. For signed graphs the adjacency matrix is defined as follows.

$$A = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if } j > i \text{ and } i \text{ and } j \text{ are neighbors} \\ -1 & \text{if } i > j \text{ and } i \text{ and } j \text{ are neighbors} \\ 0 & \text{otherwise} \end{cases} \quad (12)$$

Such graphs have many applications among which lattice statistics<sup>40</sup> in statistical mechanics is one of them. Note that the signed graphs whose adjacency matrixes are defined above are special cases of directed graphs. A signed graph could also be weighted.

It is well known that computer codes in general could have logical or other errors which are called "bugs." One needs several aids to debug codes. Debugging the code for weighted graphs was not easy since many known characteristic polynomials are effective only for ordinary graphs. However, this was useful to some level since in the limit of all weights of a weighted graph being equal to unity, the characteristic polynomial of the weighted graph is the same as the poly-

mial of the corresponding unweighted graph. This was used to reproduce the characteristic polynomials of many graphs for which the weights were read in as unities. This procedure, however, does not assure that the code is debugged.

Balasubramanian and Randić<sup>10</sup> have shown that the method of tree pruning can be applied to obtain the characteristic polynomials of edge-weighted trees. These authors have obtained the characteristic polynomials of many weighted trees. These results were used to compute the characteristic polynomials of many graphs they considered in that paper by using a few chosen nonintegral weights. All these cases were used to debug the code.

The code developed here should work without any difficulty for weighted graphs containing up to 200 vertices. However, for directed graphs since both upper and lower triangle of the adjacency matrix need to be stored more memory (approximately double) would be required. It must also be pointed out that for graphs containing large numbers of vertices if the weights of many edges

**Table V.** Characteristic polynomials of weighted "linear" chains  $L_n$  with bond alteration ( $\beta_D/\beta_S = 1.159$ ).

$n$	Characteristic Polynomial
4	$\lambda^4 - 3.6866\lambda^2 + 1.8044$
6	$\lambda^6 - 6.0298\lambda^4 + 9.0998\lambda^2 - 2.4238$
8	$\lambda^8 - 8.3731\lambda^6 + 21.8861\lambda^4 - 18.7951\lambda^2 + 3.2559$
10	$\lambda^{10} - 10.7164\lambda^8 + 40.1634\lambda^6 - 61.9806\lambda^4 + 35.0744\lambda^2 - 4.3736$
12	$\lambda^{12} - 13.0597\lambda^{10} + 63.9317\lambda^8 - 144.8473\lambda^6$ $+ 150.9132\lambda^4 - 61.3157\lambda^2 + 5.8749$
14	$\lambda^{14} - 15.4030\lambda^{12} + 93.1909\lambda^{10} - 280.2620\lambda^8$ $436.3803\lambda^6 - 331.6904\lambda^4 + 102.4401\lambda^2 - 7.8917$
16	$\lambda^{16} - 17.7462\lambda^{14} + 127.9411\lambda^{12} - 481.0917\lambda^{10} + 1007.2348\lambda^8$ $- 1159.6815\lambda^6 + 676.9650\lambda^4 - 165.5734\lambda^2 + 10.6007$
18	$\lambda^{18} - 20.0895\lambda^{16} + 168.1823\lambda^{14} - 760.2032\lambda^{12}$ $+ 2009.3862\lambda^{10} - 3143.4450\lambda^8 + 2808.2431\lambda^6$ $- 1306.3393\lambda^4 + 260.9797\lambda^2 - 14.2397$
20	$\lambda^{20} - 22.4328\lambda^{18} + 213.9144\lambda^{16} - 1130.4633\lambda^{14}$ $+ 3618.8950\lambda^{12} - 7205.7602\lambda^{10}$ $+ 8821.2186\lambda^8 - 6329.0640\lambda^6$ $+ 2412.7455\lambda^4 - 403.3771\lambda^2 + 19.1280$

is greater than unity then numerical errors due to roundoff could become significant. Even, in double precision arithmetic this error could be large in absolute sense. Thus, if the weights of many edges are greater than 1 and the graph contains more than 50 vertices, one would need to use higher precision in a 32-bit machine or use a machine such as Cray which uses a word with longer bits to store numbers. We see this as the only limitation with this or any code to compute numbers of such magnitude. Central processing unit (CPU) time is of little consideration since even for graphs containing a large number of vertices the polynomial could be obtained with very little time.

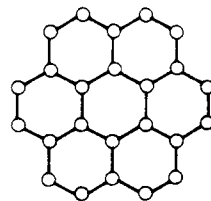
### III. RESULTS AND DISCUSSION

Table V shows the characteristic polynomials of linear weighted graphs denoted as  $L_n$ . The weights are chosen with the assumption that these chains represent conjugated hydrocarbons and the ratio of the weights for single and double bonds ( $\beta_D/\beta_S$ ) is given by the Ohno parameterization ( $\beta_D/\beta_S = 1.159$ ) as described in Ohmine et al.<sup>41</sup> for polyenes. Note that the computer code for the polynomial could take any weight and this particular choice is only used as an illustration of how the code could be used for polyenes with bond alternation. Note that the coefficient of the constant term is  $(\beta_D/\beta_S)^n$  for  $L_n$ . This can be verified using the tree pruning method.<sup>8,9</sup>

Next, we consider the graph shown in Figure 1. We allow bond alteration by choosing different weights for single and double bonds ( $\beta_D/\beta_S = 1.159$ ) in accordance with Ohmine et al.<sup>41</sup> The resulting polynomial is shown below.

$$\begin{aligned} \lambda^{24} &- 34.1194\lambda^{22} + 501.8812\lambda^{20} \\ &- 4198.5305\lambda^{18} + 22,184.3337\lambda^{16} \\ &- 77,739.0678\lambda^{14} + 184,508.0701\lambda^{12} \\ &- 297,347.4389\lambda^{10} + 320,790.8669\lambda^8 \\ &- 223,826.8456\lambda^6 + 94,569.7463\lambda^4 \\ &- 21,349.9686\lambda^2 + 1942.9424 \end{aligned} \quad (13)$$

If one substitutes one of the vertices (of valency 2) in each of the outer 6 rings in Figure 1 with nitrogen atoms such that the resulting structure preserves the  $D_{6h}$  symmetry, the resulting graph is a vertex- and edge-weighted graph if bond alteration is also included. If one chooses a weight of 0.5 for the nitrogen atom, then one obtains the



**Figure 1.** The graph of coronene. The characteristic polynomial of this structure which includes bond alteration is given by (13). The characteristic polynomial for the heterostructure obtained by substituting one vertex (of degree 2) of each of the 6 outer rings so that  $D_{6h}$  symmetry is preserved is given by (14) (weight of the heterovortex = 0.5).

following characteristic polynomial for the resulting edge- and vertex-weighted graph.

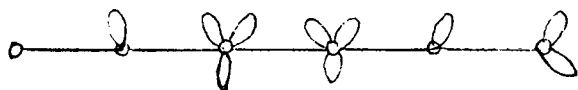
$$\begin{aligned} \lambda^{24} &- 3.0\lambda^{23} - 28.908\lambda^{22} + 84.498\lambda^{21} \\ &+ 356.064\lambda^{20} - 1112.6388\lambda^{19} \\ &- 2582.8477\lambda^{18} + 8257.338\lambda^{17} \\ &+ 11686.4272\lambda^{16} - 38,384.3447\lambda^{15} \\ &- 35,062.5022\lambda^{14} + 116,330.0209\lambda^{13} \\ &+ 70,575.369\lambda^{12} - 237,242.6538\lambda^{11} \\ &- 103,732.5719\lambda^{10} + 306,350.3708\lambda^9 \\ &+ 76,631.2727\lambda^8 - 355,663.5005\lambda^7 \\ &- 235,255.227\lambda^6 - 463,070.2832\lambda^5 \\ &- 1,141,554.8947\lambda^4 - 4,765,413.1001\lambda^3 \\ &- 8,599,306.3219\lambda^2 - 36,769,181.9104\lambda \\ &- 183,369,070.0652 \end{aligned} \quad (14)$$

We also show, for comparison, the characteristic polynomial of the graph in Figure 1 obtained earlier<sup>2</sup> without weights.

$$\begin{aligned} \lambda^{24} &- 30\lambda^{22} + 387\lambda^{20} - 2832\lambda^{18} + 13059\lambda^{16} \\ &- 39,858\lambda^{14} + 82,281\lambda^{12} - 115,272\lambda^{10} \\ &+ 108,192\lambda^8 - 65,864\lambda^6 + 24,432\lambda^4 \\ &- 4896\lambda^2 + 400 \end{aligned} \quad (15)$$

Note that the bond alteration, in general, increases the magnitude of the coefficients. The inclusion of heteroatoms gives rise to additional terms. In fact, the coefficient of  $\lambda^{n-1}$ , where  $n$  is the number of vertices in the graph is simply the sums of all the weights of the vertices since this coefficient is the trace of the adjacency matrix. Since for the heterograph of Figure 1, there are 6 nitrogen atoms with each being weighted with 0.5, this coefficient should be 3.0 in agreement with the coefficient of  $\lambda^{23}$  in expression (14).

The present code could also be used to generate the characteristic polynomials of graphs with loops. Consider the chain with loops shown in Figure 2. The adjacency matrix of such a graph would have diagonal elements being equated with the number of loops corresponding to that vertex. For example, the first diagonal element of the adjacency matrix of the graph in Figure 2 would be 0, the second diagonal being 1, third being 3, etc. The characteristic poly-



**Figure 2.** A linear chain with multiple loops. For the characteristic polynomial of this graph see (16).

nomial of this graph is given by (16)

$$\lambda^6 - 10\lambda^5 + 33\lambda^4 - 36\lambda^3 - 8\lambda^2 + 24\lambda - 2 \quad (16)$$

Next, we consider a few directed graphs. Special cases of directed graphs are signed graphs. The adjacency matrices of signed graphs were defined in Section II. Consider a class of signed graphs resulting from  $C_n$ , a cycle containing  $n$  vertices. The characteristic polynomials of these graphs are shown in Table VI for  $C_4$ – $C_{20}$  for even  $n$ . It may be tempting to conclude that the characteristic polynomial of a signed graph is the same as that of the ordinary graph but for sign. This is, in general, false as seen from Table VI. For the simplest case, namely,  $C_4$ , the polynomial for the regular graph is  $\lambda^4 - 4\lambda^2$ . The constant coefficient is 0 differing from Table VI. However, for  $C_6$  the characteristic polynomial of the regular (unsigned) graph is

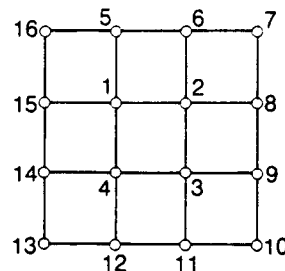
$$\lambda^6 - 6\lambda^4 + 9\lambda^2 - 4 \quad (17)$$

Thus the polynomial differs only in the signs. For the naphthalene graph, the polynomials of signed and unsigned graphs are given by expressions (18) and (19), respectively.

$$\lambda^{10} + 11\lambda^8 + 41\lambda^6 + 65\lambda^4 + 43\lambda^2 + 9 \quad (18)$$

$$\lambda^{10} - 11\lambda^8 + 41\lambda^6 - 65\lambda^4 + 43\lambda^2 - 9 \quad (19)$$

Thus for some graphs the polynomials differ only by the signs of the coefficients. Our observation is that for all graphs which are based on  $C_4$  (eq. square lattice) the polynomials of signed and unsigned graphs differ. Consider, for example, the square lattice shown in Figure 3. The ordinary characteristic polynomial of this lattice is given by (20) while for the signed lattice, the poly-



**Figure 3.** A signed square lattice. Although, directions are not shown in this figure the weight of an edge from  $i$  to  $j$  is +1 if  $j > i$  and -1 if  $j < i$ . The characteristic polynomial of this lattice is given by (20).

Table VI. Characteristic polynomials of some signed graphs  $C_n$ .

Signed Graph	Characteristic Polynomial
$C_4$	$\lambda^4 + 4\lambda^2 + 4$
$C_6$	$\lambda^6 + 6\lambda^4 + 9\lambda^2 + 4$
$C_8$	$\lambda^8 + 8\lambda^6 + 20\lambda^4 + 16\lambda^2 + 4$
$C_{10}$	$\lambda^{10} + 10\lambda^8 + 35\lambda^6 + 50\lambda^4 + 25\lambda^2 + 4$
$C_{12}$	$\lambda^{12} + 12\lambda^{10} + 54\lambda^8 + 112\lambda^6 + 105\lambda^4 + 36\lambda^2 + 4$
$C_{14}$	$\lambda^{14} + 14\lambda^{12} + 77\lambda^{10} + 210\lambda^8 + 294\lambda^6 + 196\lambda^4 + 49\lambda^2 + 4$
$C_{16}$	$\lambda^{16} + 16\lambda^{14} + 104\lambda^{12} + 352\lambda^{10} + 660\lambda^8 + 672\lambda^6 + 336\lambda^4 + 64\lambda^2 + 4$
$C_{18}$	$\lambda^{18} + 18\lambda^{16} + 135\lambda^{14} + 546\lambda^{12} + 1287\lambda^{10} + 1782\lambda^8 + 1386\lambda^6 + 540\lambda^4 + 81\lambda^2 + 4$
$C_{20}$	$\lambda^{20} + 20\lambda^{18} + 170\lambda^{16} + 800\lambda^{14} + 2275\lambda^{12} + 4004\lambda^{10} + 4290\lambda^8 + 2640\lambda^6 + 825\lambda^4 + 100\lambda^2 + 4$

mial is given by (21)

$$\lambda^{16} + 24\lambda^{14} + 226\lambda^{12} + 1064\lambda^{10} + 1888\lambda^8 + 3352\lambda^6 + 1888\lambda^4 + 320\lambda^2 + 16 \quad (20)$$

$$\lambda^{16} - 24\lambda^{14} + 206\lambda^{12} - 804\lambda^{10} + 1481\lambda^8 - 1260\lambda^6 + 400\lambda^4 \quad (21)$$

Expressions (20) and (21) differ in every coefficient except the first two terms to convince us that the polynomials of signed graphs are, in general, different from those of unsigned graphs. The graphs with four-membered rings have terms that cancel while those of six-membered rings do not. Thus the characteristic polynomials of signed and ordinary graphs for six-membered ring systems are the same. The coefficients of the polynomials of signed graphs are always positive.

## CONCLUSION

In this investigation we developed computer codes for (1) the characteristic polynomials of edge/vertex-weighted graphs and (2) the characteristic polynomials of directed and signed graphs. The characteristic polynomials of many edge/vertex-weighted graphs and directed graphs were obtained. These codes would be useful in a number of applications in chemical kinetics, lattice statistics, quantum chemistry of polymers, and unsaturated systems containing heteroatoms.

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