Energy Of Chemical Graphs With Adjacency Rhotrix

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Abstract:
For a connected graph Gthe characteristic polynomial of G is the determinant value of the matrix A(G)-λI, where A(G) is the adjacency of the matrix of G and I is the identity matrix. The roots of the characteristic polynomial equation are known as eigen values of G. The sum of the absolute values of the eigen values of G is called the energy of G and the largest eigen value is the spectral radius of G. Energies of molecular graphs have various applications in chemistry, polymerization, computer networking and pharmacy. In this paper we present the characteristic polynomial of certain graphs in terms of recurrence relation. Moreover we introduce a method to find the characteristic polynomial of a graph with single vertex deletion using adjacency Rhotrix.
Keywords:
characteristic polynomial, recurrence relation, rhotrix, coupled matrix.

1. INTRODUCTION

Let *G* be a simple connected graph on the vertex set $V(G)=\{v_1,v_2,v_3,\ldots v_n\}$. If any two vertices of a graph are connected by a line then the line is called edge of the graph *G*. The connected vertices by an edge are known as adjacent vertices. The adjacency matrix of a graph *G* is a symmetric matrix of order$n\times n$ denoted by *A(G)* and defined by $A(G)=(a_{ij})$, where $a_{ij}= 1$ if v_i and v_j are adjacent and $a_{ij}= 0$ otherwise. The characteristic polynomial of G is $\chi(G) = det(A(G)-\lambda I)$, where *I* is the identity matrix of order *n*. The spectrum *Sp(G)* is the collection of all eigen values of *A(G)*, which are real numbers because *A(G)* is a real symmetric matrix. Graph energy of G is the sum of the absolute values of eigen values of *A(G*). Graph energy is a concept transplanted from chemistry to mathematics. A chemical graph or a molecular graph can be represented by taking the vertices of a graph as atoms and edges as bonds between the atoms of chemical structure. The structural formula C_4H_8 of cyclobutane is equivalent to a cycle graph C_4 on four vertices. The structural formula of Propane is equivalent to a path graph P_3 on three vertices.

2. MATERIALS AND METHODS

In this section, we collect the basic definitions and theorems, which are needed for the subsequent sections and we refer distance in graphs by Harary (1969)[11] and graph energy by Gutman et al. (2012)[9] for basic concepts.

Mathematical arrays that are in some way between two-dimensional vectors and 2 × 2 dimensional matrices were suggested by Atanssov and Shannon (1998)[5]. As an extension to this idea, Ajibade (2003)[2] introduced an object that lies between 2 × 2 dimensional matrices and 3 × 3 dimensional matrices called ‘Rhotrix’. A Rhotrix R_3 is of the form

$$R_3 = \left\langle \begin{matrix} & a_1 & \\ a_2 & h(R_3) & a_3 \\ & a_4 & \end{matrix} \right\rangle$$

where a_1, a_2, a_3, a_4 and $h(R_3)$ are real numbers. Here, $h(R_3)$ is the heart of R_3. For any rhotrix R_n, $n \epsilon 2Z^+ + 1$. If the n dimensional rhotrix is denoted by R_n and $|R_n|$ the number of elements of R_n, then

$$|R_n| = \frac{(n^2+1)}{2}$$

A rhotrix R_n is indicated by

$$R_n = \left\langle \begin{matrix} & & & & a_{11} & & & & \\ & & & a_{21} & c_{11} & a_{12} & & & \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ a_{t1} & \dots & \dots & \dots & \dots & \dots & \dots & \dots & a_{1t} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ & & & a_{n-1} & c_{t-1t-1} & a_{t-1t} & & & \\ & & & & a_n & & & & \end{matrix} \right\rangle$$

A rhotrix R_n can also be written as $R_n = \langle (a_{ij}), (c_{kl}) \rangle$, where $\langle (a_{ij}) \rangle$ is of order $t \times t$, $\langle (c_{kl}) \rangle$ is oforder $(t-1) \times (t-1)$. Now we convert the rhotrix into coupled matrix. By rotating the columns of a rhotrix through 45°, a special form of matrix formed which is the transpose of a rhotrix. For instance to an R_5 rhotrix, we get

$$R_5^{T/2} = \left\langle \begin{matrix} & & a_{11} & & \\ & a_{21} & c_{11} & a_{12} & \\ a_{31} & c_{21} & a_{22} & c_{12} & a_{13} \\ & a_{32} & c_{22} & a_{23} & \\ & & a_{33} & & \end{matrix} \right\rangle^{T/2}$$

$$= \left\langle \begin{matrix} a_{11} & & a_{12} & & a_{13} \\ & c_{11} & & c_{12} & \\ a_{21} & & a_{22} & & a_{23} \\ & c_{21} & & c_{22} & \\ a_{31} & & a_{32} & & a_{33} \end{matrix} \right\rangle$$

Figure 1: Rhotrix R_5

In general, we have $R_n^{T/2} = \langle (a_{ij}), (c_{kl}) \rangle^{T/2} = [AC]$, which is a coupled matrix, coupling a $t \times t$ matrix with a $(t-1) \times (t-1)$ matrix where $t = \frac{(n+1)}{2}$. A coupled matrix $[(a_{ij}), (c_{kl})]$ is called filled coupled matrix if $a_{ij} = 0, \forall i, j$ whose aggregation ($i+ j$) is odd. For example the coupled matrix in Figure 1 becomes a filled coupled matrix as below.

$$\begin{bmatrix} a_{11} & 0 & a_{12} & 0 & a_{13} \\ 0 & c_{11} & 0 & c_{12} & 0 \\ a_{21} & 0 & a_{22} & 0 & a_{23} \\ 0 & c_{21} & 0 & c_{22} & 0 \\ a_{31} & 0 & a_{32} & 0 & a_{33} \end{bmatrix}$$

Definition 2.1:

The adjacency rhotrix of G is a coupled matrix of adjacency matrices of $G$and $G – v$.

Example 2.2:Let $G = K_4$. Then $G – v = K_3$. The adjacency rhotrix of K_4 is

$$R_5 = \left\langle \begin{array}{ccccccc} & & & 0 & & & \\ & & 1 & 0 & 1 & & \\ & 1 & 1 & 0 & 1 & 1 & \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ & 1 & 1 & 0 & 1 & 1 & \\ & & 1 & 0 & 1 & & \\ & & & 0 & & & \end{array} \right\rangle$$

$$= \left\langle \begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{bmatrix} \right\rangle$$

$$= \langle \mathrm{A(K_4), A(K_3)} \rangle$$

Filled coupled matrix of R_4 is

$$\begin{bmatrix} 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 \end{bmatrix}$$

3. MAIN RESULTS

In this section, the recurrence relation for characteristic polynomial of certain graphs are presented.

Algorithm to find the recurrence relation of characteristic polynomial, spectrum and energy of graph.

Step 1 Draw a graph G of order n∈Nunder consideration with proper labelling.

Step 2 Write $A(G)$, the adjacency matrix of G.

Step 3 Find $|A(G) – \lambda I|$ which gives G's characteristic polynomial.

Step 4 Find spectrum of G, the collection of all characteristic roots of $|A(G) – \lambda I| = 0$.

Step 5 Find energy of G, the aggregate of the absolute values of characteristic roots of

$|A(G) - \lambda I| = 0$.

Step 6 Find the spectral radius of G, which is the dominant eigenvalue.

Algorithm to find the energy of both G and G – v by adjacency rhotrix.

Step 1 Write adjacency matrix $A(G)$ called major matrix, of order equal to order of $G$and adjacency matrix $A(G - v)$ called minor matrix, where $G - v$ is one vertex deleted connected induced sub graph of G.

Step 2 Write the rhotrixR_p, where $p = 2n - 1$ with major matrix as $A(G)$ and minor matrix as $A(G - v)$.

Step 3 Write the coupled matrix of R_p.

Step 4 Write the filled coupled matrix of R_p.

Step 5 Find the eigenvalues of filled coupled matrix using MATLAB program. Let the eigenvalues be $\lambda_1, \lambda_2, \lambda_3, \lambda_4, \lambda_5, \lambda_6, \ldots, \lambda_{2n-2}, \lambda_{2n-1}$. The values $\lambda_1, \lambda_3, \lambda_5, \ldots, \lambda_{2n-1}$are the eigenvalues of G and $\lambda_2, \lambda_4, \lambda_6, \ldots, \lambda_{2n-2}$are eigenvalues of $G - v$.

Definition 3.1:

A Y-tree is a graph obtained from path graph P_n, $n \geq 3$ by appending avertex with Pendant edge of a path adjacent to an end vertex. It is denoted by YP_n.

Definition 3.2:

A F-tree is a graph obtained from path graph P_n, $n \geq 3$ by appending twoPendant edges one to an end vertex of a path and the other to a vertex adjacent to an endvertex. It is denoted by FP_n.

Definition 3.3:

A E-tree is a graph obtained from path graph P_n, $n \geq 4$ by appending threePendant edges to the first three vertices of $P_n$or the last three vertices of P_n.

Theorem 3.4:

If $G = YP_n$is a Y-tree then the characteristic polynomial of $YP_n$for $n \geq 5$ is
$\chi(YP_n, \lambda) = -\lambda\chi(Y P_3, \lambda) - \chi(Y P_{n-2}, \lambda)$, where $\chi(Y P_4, \lambda) = -\lambda^5 + 4\lambda^3 - 2\lambda$and
$\chi(Y P_3, \lambda) = \lambda^4 - 3\lambda^2$.

*Proof***:**

Let $V(G) = \{u_1, u_2, \ldots, u_n, v\}$ and $E(G) = \{u_i\ u_{i+1};\ 1 \leq i \leq n - 1\} \cup \{u_{n-1}v\}$ of YP_ntree, respectively. Here, the pendant edge is$v\ u_{n-1}$. We first find the characteristicpolynomial of YP_3.

The graph $G = YP_3$ is shown in Figure 2.

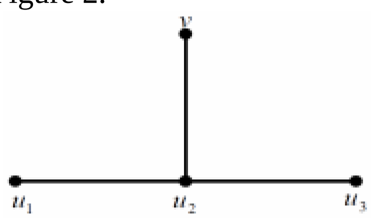

Figure 2 YP_3

The adjacency matrix $A(G)$ is given by

$$A(G) = \begin{array}{c} \\ u_1 \\ u_2 \\ u_3 \\ v \end{array} \begin{array}{c} \begin{array}{cccc} u_1 & u_2 & u_3 & v \end{array} \\ \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

The characteristic polynomial of *G* is

$$\chi(\mathrm{G}) = |\mathrm{A(G)} - \lambda \mathrm{I}|$$

$$= \begin{vmatrix} -\lambda & 1 & 0 & 0 \\ 1 & -\lambda & 1 & 1 \\ 0 & 1 & -\lambda & 0 \\ 0 & 1 & 0 & -\lambda \end{vmatrix}$$

$$= \lambda^4 - 3\lambda^2$$

Let $G = YP_4$.

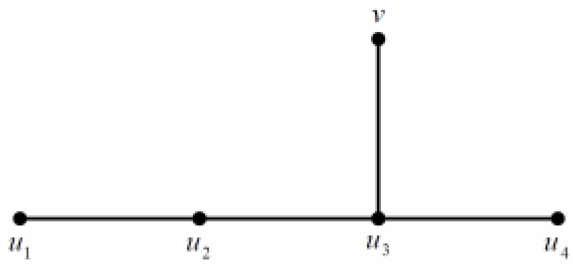

Figure 3 $Y\,P_4$

The adjacency matrix $A(G)$ is given by

$$A(G) = \begin{array}{c} \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ v \end{array} \begin{array}{c} \begin{array}{ccccc} u_1 & u_2 & u_3 & u_4 & v \end{array} \\ \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

The characteristic polynomial of *G* is

$$\chi(\mathrm{G}) = |\mathrm{A(G)} - \lambda \mathrm{I}|$$

$$= \begin{vmatrix} -\lambda & 1 & 0 & 0 & 0 \\ 1 & -\lambda & 1 & 0 & 0 \\ 0 & 1 & -\lambda & 1 & 1 \\ 0 & 0 & 1 & -\lambda & 0 \\ 0 & 0 & 1 & 0 & -\lambda \end{vmatrix}$$

$$= -\lambda^5 + 4\lambda^3 - 2\lambda$$

The characteristic polynomial of $A(YP_5)$ is

$$\chi(A(YP_5), \lambda) = \lambda^6 - 5\lambda^4 + 5\lambda^2$$

$$= -\lambda(-\lambda^5 + 4\lambda^3 - 2\lambda) - (\lambda^4 - 3\lambda^2)$$

$$= -\lambda\chi(A(YP_4), \lambda) - \chi(A(YP_3), \lambda)$$

Hence, the recurrence relation of characteristic polynomial of $A(YP_n)$ for $n \geq 5$ is

$\chi(A(YP_n), \lambda) = -\lambda\chi(YP_{n-1}, \lambda) - \chi(YP_{n-2}, \lambda)$, where $\chi(YP_4, \lambda) = -\lambda^5 + 4\lambda^3 - 2\lambda$ and $\chi(YP_n, \lambda) = \lambda^4 - 3\lambda^2$.

Theorem 3.5:

If FP_n is a F tree obtained from P_n, then $\chi(FP_n, \lambda) = -\lambda\chi(FP_{n-1}, \lambda) - \lambda\chi(FP_{n-2}, \lambda)$ where $\chi(FP_3, \lambda) = -\lambda^5 + 4\lambda^3 - 2\lambda$ and $\chi(FP_4, \lambda) = -\lambda^6 + 5\lambda^4 - 5\lambda^2 + 1$.

Proof:

Let $G = FP_n$ be a F-tree obtained from path graph P_n with $V(G) = \{u_1, u_2, u_3, u_4, \ldots, u_n, v, w\}$ and $E(G) = \{u_i u_{i+1}; 1 \leq i \leq n-1\} \cup \{u_n w, u_{n-1} v\}$. Here, $u_n w$ and $u_{n-1} v$ are thependant edges. We first find the characteristic polynomial FP_3. The graph FP_3 is given inFigure 4.

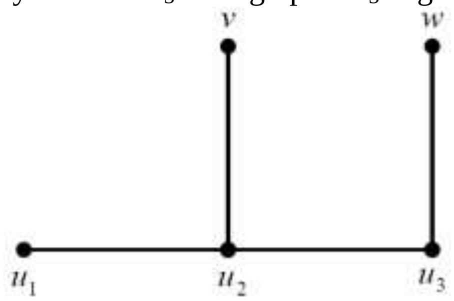

Figure 4 FP_3

The adjacency matrix $A(G)$ is given by

$$A(G) = \begin{array}{c} \\ u_1 \\ u_2 \\ u_3 \\ v \\ w \end{array} \begin{array}{c} \begin{array}{ccccc} u_1 & u_2 & u_3 & v & w \end{array} \\ \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

The characteristic polynomial of G is

$$\chi(\mathrm{G}) = |\mathrm{A(G)} - \lambda \mathrm{I}|$$

$$= \begin{vmatrix} -\lambda & 1 & 0 & 0 & 0 \\ 1 & -\lambda & 1 & 1 & 0 \\ 0 & 1 & -\lambda & 0 & 1 \\ 0 & 1 & 0 & -\lambda & 0 \\ 0 & 0 & 1 & 0 & -\lambda \end{vmatrix}$$

$$= -\lambda \begin{vmatrix} -\lambda & 1 & 1 & 0 \\ 1 & -\lambda & 0 & 1 \\ 1 & 0 & -\lambda & 0 \\ 0 & 1 & 0 & -\lambda \end{vmatrix} - \begin{vmatrix} 1 & 1 & 1 & 0 \\ 1 & -\lambda & 0 & 1 \\ 0 & 0 & -\lambda & 0 \\ 0 & 1 & 0 & -\lambda \end{vmatrix}$$

$$= (-\lambda)(-\lambda) \begin{vmatrix} -\lambda & 1 & 1 \\ 1 & -\lambda & 0 \\ 1 & 0 & -\lambda \end{vmatrix} - \lambda \begin{vmatrix} -\lambda & 1 & 1 \\ 1 & 0 & -\lambda \\ 0 & 1 & 0 \end{vmatrix} - \begin{vmatrix} -\lambda & 0 & 1 \\ 0 & -\lambda & 0 \\ 1 & 0 & -\lambda \end{vmatrix}$$

$$= \lambda^2[-\lambda(\lambda^2 - 1) + \lambda] - \lambda[-(\lambda^2 - 1)] - [-\lambda(\lambda^2) + \lambda]$$

$$= \lambda^2[\lambda^3 + \lambda + \lambda] + (\lambda^3 - \lambda) + \lambda^3 - \lambda$$

$$= -\lambda^5 + 2\lambda^3 + 2\lambda^3 - 2\lambda$$

$$= -\lambda^5 + 4\lambda^3 - 2\lambda$$

By expanding the adjacency matrices of FP_4 tree and FP_5 tree, we get the following characteristic polynomials.

$$\chi(FP_4, \lambda) = \lambda^6 - 5\lambda^4 + 5\lambda^2 - \lambda$$

$$\chi(FP_5, \lambda) = -\lambda^7 + \lambda^5 - 9\lambda^3 + 3\lambda$$

$$= -\lambda(\lambda^6 - 5\lambda^4 + 5\lambda^2 - \lambda) - (-\lambda^5 + 4\lambda^3 - 2)$$

$$= -\lambda\chi(FP_4, \lambda) - \chi(FP_3, \lambda)$$

Therefore for $n \geq 5$, the recurrence relation for characteristic polynomial of $FP_n$is
$\chi(FP_n, \lambda) = -\lambda\chi(FP_{n-1}, \lambda) - \lambda\chi(FP_{n-2}, \lambda)$.

Theorem 3.6:

Let G=EP$_n$be the E tree. Then the characteristic polynomial of G
as $\chi(EP_n, \lambda) = -\lambda\chi(FP_{n-1}, \lambda) - \chi(P_{n-2}, \lambda)$ where $\chi(EP_4, \lambda) = -\lambda^7 + 6\lambda^5 - 8\lambda^3 + 2\lambda$ and
$\chi(EP_5, \lambda) = \lambda^8 - 7\lambda^6 + 13\lambda^4 - 7\lambda^2 + 1$ for $n \geq 6$.

4. CHARACTERISTIC POLYNOMIAL OF COMB-LIKE GRAPH

Let $V(C_n) = \{u_1, u_2, \ldots, u_n\}$ be the vertex set of a n vertices cycle graph with u_1 as the start vertex and $u_n$as the end vertex. If the n vertices $v_1, v_2, \ldots, v_n$are attached to each vertex of $C_n$we get the n pendant edges $u_i\, v_i$; $1 \leq i \leq n$ and we call the pendant edges $u_iv_i$as teeth. The cycle graph C_n with n teeth is denoted by $G_n = (C_n: v_1, v_2, \ldots, v_n)$ for $n \geq 3$ and this graph G_n is called circular comb on n vertices. If the circular comb has exactlyone tooth say u_1v_1 then it is denoted byG_n^1=(C_n: v_1) and with two teeth $u_1\, v_1$, $u_2\, v_2$,then it is denoted byG_n^2=(C_n: v_1, v_2) and so on. In general a circular comb with $i$teeth$u_1\, v_1, u_2\, v_2, \ldots, u_i\, v_i$is denoted by G_n^i=(C_n: v_1, $v_2, \ldots v_i$).A circular comb
$G_7^5 = (C_7: v_1, v_2, \ldots v_5)$ is shown in Figure 5.

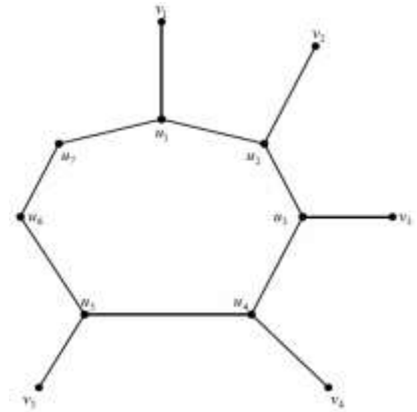

Figure 5G_7^5

Definition 4.1:

An $n \times n$ circulant matrix C is defined as

$$\mathrm{C} = \begin{bmatrix} c_0 & c_{n-1} & \cdots & \cdots & c_2 & c_1 \\ c_1 & c_0 & c_{n-1} & \cdots & \cdots & c_2 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ c_{n-2} & \cdots & \cdots & \cdots & \cdots & c_{n-1} \\ c_{n-1} & c_{n-2} & \cdots & \cdots & c_1 & c_0 \end{bmatrix}$$

The eigenvalues of circulant matrix are $\lambda_j = c_0 + c_{n-1}w^j + c_{n-2}w^{2j} + \ldots + c_1 w^{(n-1)j}$, $j = 0, 1, 2, \ldots, n - 1$,

$w^j = \exp\left[\frac{2\pi ij}{n}\right]$ gives the n^th^ roots of unity. The C_n spectrum is $Sp(C_n)\{\cos\left[\frac{2\pi j}{n}\right], j = 1, 2, \ldots n\}$. The spectrum of P_n is $Sp(P_n) = \{2cps\left[\frac{\pi j}{n+1}\right], j = 1, 2, \ldots n\}$.

Theorem 4.2:

Let G_n^n=(C_n: v_1, v_2,…v_n)be the circular comb of $2n$ vertices. Then the characteristic polynomial of is G_n^n is

$$\chi((C_n; v_1, v_2, \ldots, v_n), \lambda) = [\chi(P_n, \lambda) - \chi\lambda(P_n, \lambda) + \chi\lambda^2(P_n, \lambda) + \ldots + (-1)^{n-1}\chi\lambda^{n-1}(P_n, \lambda) + (-1)^{n-1}\chi(c_n, \lambda)$$

Proof:

Let $V(G_n^n)$={u_1, u_2,…, u_n}∪{v_1, v_2,…, v_n}and $E(G_n^n)$={u_iu_{i+1}, $1 \le i \le n - 1$}∪{u_1 v_1 }∪{u_i v_i: $1 \le i \le n$}. Let G_n^1=(C_n;v_1).

The adjacency matrix of (C_n;v_1) is

$$A[C_n;v_1] = \begin{array}{c} \\ u_1 \\ u_2 \\ u_3 \\ \cdots \\ \cdots \\ \cdots \\ u_{n-1} \\ u_n \\ v_1 \end{array} \begin{array}{c} \begin{array}{ccccccccc} u_1 & u_2 & u_3 & \cdots & \cdots & \cdots & u_{n-1} & u_n & v_1 \end{array} \\ \begin{pmatrix} 0 & 1 & 0 & \cdots & \cdots & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & \cdots & \cdots & \cdots & 0 & 0 & 0 \\ 0 & 1 & 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & \cdots & \cdots & \cdots & 1 & 0 & 0 & 0 \\ 1 & 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

Expanding the $|A(C_n: v_1), \lambda|$ we get the characteristic polynomial of $A(C_n: v_1)$ is $\chi((C_n: v_1), \lambda) = -\lambda\chi(C_n, \lambda) + \chi(P_n, \lambda)$ where $\chi(C_n, \lambda)$ is a characteristic polynomial of cycle graph $C_n$and $\chi(P_n, \lambda)$ is a characteristic polynomial of path graph P_n. Proceeding similarly, we get

$$\begin{aligned}
\chi((C_n;v_1,v_2),\lambda) &= -\chi\lambda((C_n,v_1),\lambda) + \chi(P_n,\lambda) \\
&= -\lambda[-\chi\lambda(C_n,\lambda) + \chi(P_n,\lambda)] + \chi(P_n,\lambda) \\
&= \chi\lambda^2(C_n,\lambda) - \chi\lambda(P_n,\lambda) + \chi(P_n,\lambda) \\
\chi((C_n;v_1,v_2,v_3),\lambda) &= -\chi\lambda((C_n,v_1,v_2),\lambda) + \chi(P_n,\lambda) \\
&= \chi\lambda^3(C_n,\lambda) - \chi\lambda^2(P_n,\lambda) - \chi\lambda(P_n,\lambda) \\
&= \chi\lambda^2(C_n,\lambda) - \chi\lambda(P_n,\lambda) + \chi(P_n,\lambda) \\
\chi((C_n;v_1,v_2,v_3,v_4),\lambda) &= \chi\lambda^4(C_n,\lambda) - \chi\lambda^3(P_n,\lambda) + \chi\lambda^2(P_n,\lambda) \\
&= -\chi\lambda(P_n,\lambda) + \chi(P_n,\lambda)
\end{aligned}$$

Hence, for G_n^n graph, the characteristic polynomial is given by

$$\chi((C_n;v_1,v_2,...,v_n),\lambda) = [\chi(P_n,\lambda) - \chi\lambda(P_n,\lambda) + \chi\lambda^2(P_n,\lambda) + ... + (-1)^{n-1}\chi\lambda^{n-1}(P_n,\lambda) + (-1)^{n-1}\chi(c_n,\lambda)$$

Algorithm to determine the eigenvalues of a graph by adjacency rhotrix.

Let G be a given n vertices connected graph.

Input: n, $n-1$, adjacency list of connected graph G and $G - v$.

Output: Adjacency rhotrix or filled coupled matrix and eigenvalues of G and $G - v$.

Step 1 Determine the adjacency matrix using the adjacency list of G and denote it by$A = a(i, j)$.

Step 2 Determine the adjacency matrix using the adjacency list of $G - v$ and denote it by $C = c(i, j)$.

Step 3 Write the adjacency rhotrix$R = \langle A, C\rangle$.

Step 4 Write the coupled matrix and filled coupled matrix of R.

The advantage of applying this algorithm is that the eigenvalues of a graph and its onevertex deleted subgraph can be got in a single program with less execution time.

MATLAB program output in the calculation of eigenvalues with adjacency rhotrixfor the graph $(C_5:v_1)$.

```
>> A = [0 1 0 0 1 1; 1 0 1 0 0 0;
0 1 0 1 0 0; 0 0 1 0 1 0;
1 0 0 1 0 0; 1 0 0 0 0 0]
```

```
>> B = [0 1 0 0 1; 1 0 1 0 0; 0 1 0 1 0;
        0 0 1 0 1; 1 0 0 1 0]

>> R = [0 0 1 0 0 0 0 0 1 0 1;
        0 0 0 1 0 0 0 0 0 1 0;
        1 0 0 0 1 0 0 0 0 0 0;
        0 1 0 0 0 1 0 0 0 0 0;
        0 0 1 0 0 0 1 0 0 0 0;
        0 0 0 1 0 0 0 1 0 0 0;
        0 0 0 0 1 0 0 0 1 0 0;
        0 0 0 0 0 1 0 0 0 1 0;
        1 0 0 0 0 0 1 0 0 0 0;
        0 1 0 0 0 0 0 1 0 0 0;
        1 0 0 0 0 0 0 0 0 0 0]

>>eig(R)
```

-1.8608, -1.6180,-1.6180, -1.6180,-0.2541,
0.6180, 0.6180, 0.6180, 1.0000, 2.0000, 2.1149

From the set of eigenvalues of R, we can read the values of G_n^1 as

-1.8608, -1.6180, -0.2541, 0.6180, 1.0000, 2.1149

And eigenvalues of C_5 as

-1.6180, -1.6180, 0.6180, 0.6180, 2.0000

The characteristic polynomial of $G_n^1$is

>>charpoly(A)

$\lambda^6 - 6\lambda^4 + 8\lambda^2 - 2\lambda - 1$

The characteristic polynomial of $C_5$is

>>charpoly(B)

$\lambda^5 - 5\lambda^3 + 5\lambda - 2$

5. CONCLUSIONS

The paper computes the recurrence relation of characteristic polynomials of *Y*, *F*, *E* trees and circular comb graphs and its one vertex deleted subgraphs. Using MATLAB program one can get the energy of respective graphs. These results are helpful for chemists, who are doing research in organic chemistry since the graphs that are handled in this paper are some chemical graphs.

REFERENCES

[1]. Adiga, C., Balakrishnan, R. and So, W. (2010) 'The skew energy of a digraph', Linear Algebra Appl., Vol. 432, pp.1825–1835.

[2]. Ajibade, A.O. (2003) 'The concept of rhotrix in mathematical enrichment', International Journal of Mathematical Education in Science and Technology, Vol. 34, No. 2, pp.175–179.

[3]. Aminu, A. (2010a) 'The equation Rnx = b over rhotrices', International Journal of Mathematical Education in Science and Technology, Vol. 41, No. 1, pp.98–105, DOI: 10.1080/00207390903189187.

[4]. Aminu, A. (2010b) 'Rhotrix vector spaces', International Journal of Mathematical Education in Science and Technology, Vol. 41, No. 4, pp.531–573, DOI: 10.1080/00207390903398408.

[5]. Atanssov, K.T. and Shannon, A.G. (1998) ‘Matrix – tertions and matrix – noitrets exercise for mathematical enrichment’, International Journal of Mathematical Education in Science and Technology, Vol. 29, No. 6, pp.898–903.
[6]. Chen, X., Hou, Y. and Li, J. (2016) ‘On two energy-like invariants of line graphs and related graph operations’, Journal of Inequalities and Applications, Vol. 51, 15pp.
[7]. Gutman, I. (1978) ‘The energy of a graph’, Steiermark, Math. Symp., Vol. 103, pp.1–22.
[8]. Gutman, I. and Furkula, B. (2017) ‘Survey of graph energies’, Mathematics Interdisciplinary Research, Vol. 2, pp.85–129.
[9]. Gutman, I., Polansky, O. E., Mathematical Concepts in Organic Chemistry, Springer-Verlag, Berlin (1986).
[10]. Gutman, I. and Zhou, B. (2006) ‘Laplacian energy of a graph’, Linear Algebra Appl., Vol. 414, pp.29–37.
[11]. Harary, F., Graph Theory, Addison-Wesley Publishing Company, Inc., Reading, Mass., (1969).
[12]. Indulal, G. and Vijaykumar, A. (2007) ‘Energies of some non-regular graphs’, J. Math. Chem., Vol. 42, pp.377–386.
[13]. Liu, J-B. et al. (2019) ‘Distance and adjacency energies of multi-level wheel networks’, Mathematics, Vol. 7, p.43, 9pp.
[14]. Mohammed, A. (2007) ‘Enrichment exercises through extension to rhotrices’, International Journal of Mathematical Education in Science and Technology, Vol. 38, No. 1, pp.131–136,DOI: 10.1080/00207390600838490.
[15]. Mohammed, A. (2011) Theoretical Development and Applications of Rhotrices, PhD thesis, Ahmadu Bello University, Zaria.
[16]. Sani, B. (2004) ‘An alternative method for multiplication of rhotrices’, International Journal of Mathematical Education in Science and Technology, Vol. 35, No. 5, pp.777–781, DOI: 10.1080/00207390410001716577.
[17]. Sani, B. (2007) ‘The row-column multiplication of higher dimensional rhotrices’, International Journal of Mathematical Education in Science and Technology, Vol. 38, No. 5, pp.657–662.
[18]. Sani, B. (2008) ‘Conversion of a rhotrix to a coupled matrix’, International Journal of Mathematical Education in Science and Technology, Vol. 39, No. 2, pp.244–249, DOI: 10.1080/00207390701500197.
[19]. Shparlinski, I. (2006) ‘On the energy of some circulant graphs’, Linear Algebra and its Applications, Vol. 414, No. 1, pp.378–382.
[20]. Wang, W-H. and Wasin, S.O. (2015) ‘Graph energy change due to any single edge deletion’,Electronic Journal of Linear Algebra, Vol. 29, pp.50–73.