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ORIGINAL PAPER

Characteristic polynomials of alternant edge weighted linear chains with subsequent application to some linear poly (*p*-phenylene) graphs

Piyali Ghosh · Bholanath Mandal

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Abstract The algorithms for the calculation of the characteristic polynomial coefficients for the alternant edge weighted graphs of linear chains have been developed. These algorithms have been utilized to calculate the characteristic polynomials of the linear poly (*p*-phenylene) and the methylene substituted linear poly (*p*-phenylene) compounds. These compounds are found to be important materials for electro-optical and electronic applications. The recurrence relation to obtain the sum of the CP coefficients $\left(S_{\mathrm{CP}}^{N_r}\right)$ of any such poly (*p*-phenylene) in terms of the respective sums of its lower analogs has been derived. The number of Kekulé valence structures (K) for such molecular graphs have been presented. Excellent linear correlations of logarithm of sum of CP coefficients ($\log S_{\mathrm{CP}}^{N_r}$) and logarithm of Kekulé valence structures count (log K) with the ambient conditions density and bulk modulus of linear poly (*p*-phenylene) have also been found.

Keywords Characteristics polynomials · Alternant edge weighted linear chains · Linear poly (*p*-phenylene) · Kekulé valence structures · Ambient conditions density and bulk modulus

1 Introduction

The characteristic polynomial (CP) is the expanded form of the determinant $|x\mathbf{I} - \mathbf{A}|$ and is written in the form,

$$P(G; x) = |x\mathbf{I} - \mathbf{A}| = a_0 x^N + a_1 x^{N-1} + a_2 x^{N-2} + \cdots + a_N \tag{1}$$

P. Ghosh · B. Mandal (✉)
Department of Chemistry, The University of Burdwan, Burdwan 713104, India
e-mail: bmandal_05@yahoo.com

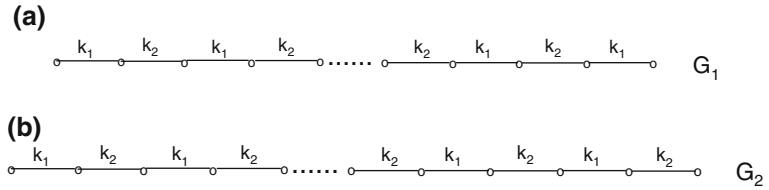


Fig. 1 Graphs of **a** even and **b** odd vertex linear chains with alternant edge weights (k_1, k_2)

where **A** is the adjacency matrix of graph and **I** is the unit matrix of the size of **A**. It is one of the basic graph invariants and the search of a variety of algorithms for its determination has been the focus of interest for a long time. Although there are a large number of algorithms [1–14] for the calculation of the CP coefficients but few of them are devoted to that for the weighted graphs [10–14]. A "weighted graph" is one that has at least one edge of weight other than 1 or a vertex of weight other than 0.

In the present paper algorithms to construct CP coefficients for the graphs of linear chains with alternant edge weights (shown in Fig. 1) have been developed that have subsequently been expressed in the form of asymmetric Pascal's triangle (PT). Pascal's triangle (PT) approach reflects the recursive relations in a much simpler manner that exists among the elements arranged in the PT. Hosoya [15,16] showed the utility of symmetric and asymmetric PTs in the enumeration of the atomic orbital wave functions of the H-atom in the general D-dimensional hyperspace. Recently simple manipulation of PT [17] has been utilized to determine the CP coefficients of reciprocal graphs (graphs having reciprocal pairs of eigenvalues), and subsequently a more direct procedure has been developed to express such coefficients in terms of the number of pendant vertices [18]. The developed algorithms in the present work have directly been used to calculate the CP coefficients of graphs of linear poly (*p*-phenylene) and the methylene substituted linear poly (*p*-phenylene) compounds. There are no such algorithms for the direct calculation of the CP coefficients of the graphs of linear chains with alternant edge weights as well as that for the above mentioned poly aromatic polymers. The beauty of this work is that the developed algorithms can easily be utilized to calculate the CP coefficients of graphs of linear poly (*p*-phenylene) and the methylene substituted linear poly (*p*-phenylene) compounds with the use of paper-pencil only. The CP coefficients of such graphs have been found to be useful to predict the structure property relationships of the corresponding molecules.

2 Characteristic polynomials of alternant edge weighted graphs of linear chains

The alternant edge weighted graphs of linear chains are of two types; even vertex chain where both the starting and the ending edges are of equal weight and the odd vertex chain where both the starting and ending edges are of different weights. Graphs with alternant edge weights represent real molecular systems; may be the systems of conjugated hetero-carbons or the subgraphs obtained from fragmentations of real molecular graphs.

2.1 Alternant edge weighted graphs of linear chains with even number of vertices

An even vertex graph (G_1) of linear chain with alternant edge weights is shown in Fig. 1a. The number of edges of such graphs of N vertices is $N-1$. Let k_1 and k_2 are the edge weights that alternate along the chain. For such graphs two terminal edges are of same weight. If the starting edge is of the weight k_1, then the number of edges of weight $k_1$is $N/2$ and that of weight k_2 is $(N-2)/2$. The characteristic polynomial of such graph can be calculated by a number of procedures [13,14]. The most convenient of these procedures is the stepwise generation of CP for a specific graph. If P_N is the characteristic polynomial of this graph, then P_N can be written [13,14] as

$$\begin{aligned} P_N &= x\,P_{N-1} - k_1^2 P_{N-2} \\ &= x^2 \sum_{i=0}^{(N-2)/2} \left(-k_2^2\right)^i P_{N-2(i+1)} - k_1^2 P_{N-2}. \end{aligned} \tag{2}$$

Assuming $P_0 = 1$ all other P_i can be calculated with the use of Eq. (2). The CP coefficients of such graphs can also be expressed in an analytical form with the help of Eq. (2) as discussed below. Let $a_{2j}^{(N)}$is the $2j$ th CP coefficient of the graph G_1, j ranges from 0 to $N/2$. Expressing CP in terms of $a_{2j}^{(N)}$ for such a graph of N vertices we obtain

$$a_{2j}^{(N)} = k_1^2 a_{2(j-1)}^{(N-2)} + \sum_{l=0}^{j} \left(k_2^2\right)^l a_{2(j-l)}^{(N-2(l+1))}. \tag{3}$$

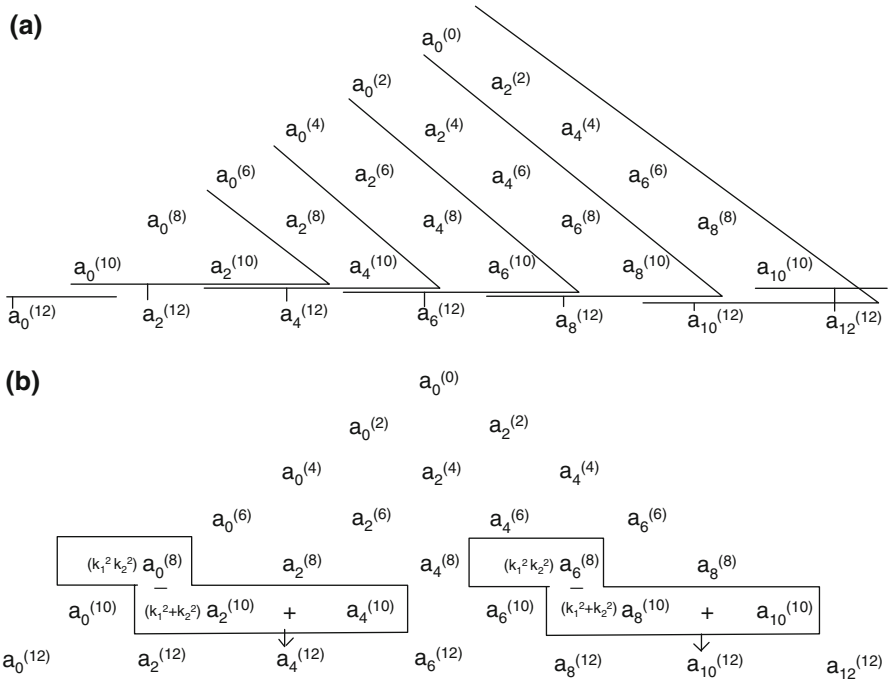
where $a_0^{(0)} = 1, a_{2j}^{(N)} = 1$ for $j = 0$ and $a_{2j}^{(N)} = 0$ for $j > N/2$. The values of j and N can not be negative and if so $a_{2j}^{(N)} = 0$.

Though the Eq. (3) resembles as recurrence relation involving coefficients of any graph with that of its lower analogues but it is really an analytical formula that may be used directly to calculate any coefficient of such a graph of N vertices.

The summation on the right hand side of the Eq. (3) is the sum of the coefficients $a_{2(j-1)}^{(N-2)}$ over l(l ranges from 0 to j with increment 1 for each term) multiplied by $\left(k_2^2\right)^l$ i.e., multiplied by the respective power of k_2^2. Thus if all the coefficients are arranged in the PT it can easily be shown that the coefficients under the summation are nothing but the elements that lie on a particular slanting column (depending on j) of the PT inclined to the left. This may easily be visualized from the illustration given in the Scheme 1a.

Thus we may write

$$\begin{aligned} a_{2j}^{(N)} = k_1^2 a_{2(j-1)}^{(N-2)} + (&\text{Sum of the CP coefficients starting from } a_{2(j-1)}^{(N-2)} \text{ on the slanting} \\ &\text{column of the PT inclined to the left multiplied by } \left(k_2^2\right)^l; l \text{ ranges} \\ &\text{from 0 to } j \text{ with increment 1 for each term}). \end{aligned} \tag{4}$$



Scheme 1 **a** Illustration for the generation of the CP coefficients of alternant edge weighted graphs of linear chains having even number of vertices. **b** Illustration for the generation of the CP coefficients (i.e., $a_4^{(12)}$ and $a_{10}^{(12)}$) of the alternant edge weighted graphs of linear chains of even number of vertices

The evaluation of the sum in the last part of the Eq. (4) becomes more and more tedious as the number of terms in the summation increases with increase in the number of vertices for such graphs. This difficulty for larger graphs can be surmounted by reducing the number of terms with proper rearrangement of Eq. (3) as

$$\begin{aligned} a_{2j}^{(N)} &= k_1^2 a_{2(j-1)}^{(N-2)} + \sum_{l=0}^{j} \left(k_2^2\right)^l a_{2(j-l)}^{(N-2(l+1))} \\ &= \left(k_1^2 + k_2^2\right) a_{2(j-1)}^{(N-2)} + a_{2j}^{(N-2)} - k_1^2 k_2^2 a_{2(j-2)}^{(N-4)} \end{aligned} \tag{5}$$

The Eq. (5) is much more convenient to calculate the CP coefficients of such a graph from the CP coefficients of its lower analogues arranged in an asymmetric PT array. For the calculation of $a_{2j}^{(N)}$, it is required to multiply $a_{2j-2}^{(N-2)}$ by $(k_1^2 + k_2^2)$, to add with $a_{2j}^{(N-2)}$ and then to subtract $a_{2j-2}^{(N-4)}$ multiplied by $(k_1^2 k_2^2)$ from this sum. This procedure is illustrated with the evaluation of two CP coefficients $a_4^{(12)}$ and $a_{10}^{(12)}$ in the Scheme 1b.

2.2 Alternant edge weighted graphs of linear chains with odd number of vertices

In Fig. 1b such a graph (G_2) of linear chain with N' number of vertices having alternant edge weights (k_1, k_2) has been shown; weight of first edge is k_1 and that of the last edge is k_2. Number of edges of weight k_1 and k_2 is same and is equal to $(N'-1)/2$. Let the characteristic polynomial of this graph is $P_{N'}$, then as discussed in Sect. 2.1, $P_{N'}$ can be written [13,14] as

$$P_{N'} = x^2 \sum_{i=0}^{(N'-3)/2} \left(-k_2^2\right)^i P_{N'-2(i+1)} + \left(-k_2^2\right)^{(N'-1)/2} x - k_1^2 P_{N-2} \tag{6}$$

Assuming $P_1 = x$, one can calculate the CP of any of such graph directly with the help of Eq. (6). In order to avoid the monotonous calculations for such a graph with large number of vertices it is convenient to use the CPs of its lower analogues. The formula for evaluation of the CP coefficients of such graphs can also be obtained from the Eq. (6). Let $a_{2j}^{(N')}$ is the $2j$th CP coefficient of such graph of N' vertices (j ranges from 0 to $(N'-1)/2$), then $a_{2j}^{(N')}$ can be expressed as

$$a_{2j}^{(N')} = k_1^2 a_{2(j-1)}^{(N'-2)} + \sum_{l=0}^{j} \left(k_2^2\right)^l a_{2(j-l)}^{(N'-2(l+1))} + \delta_{(2j)(N'-1)} k_2^{(N'-1)} \tag{7}$$

where $a_0^{(0)} = 1$, $a_{2j}^{(N')} = 1$ for $j = 0$ and $a_{2j}^{(N')} = 0$ for $j > (N'-1)/2$. The values of j and N' can not be negative and if so $a_{2j}^{(N')} = 0$.

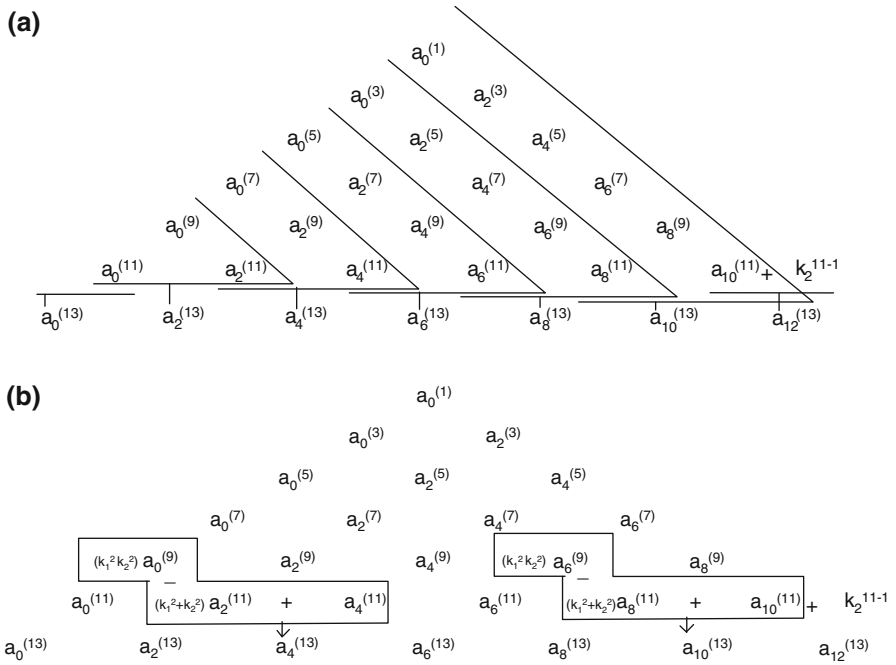
The Eq. (7) will also be used to calculate the CP coefficients of any such graph in a similar manner as has been shown in Sect. 2.1. The summation on the right hand side of the Eq. (7) represents the sum of the coefficients $a_{2(j-1)}^{(N'-2(l+1))}$ multiplied by $(k_2^2)^l$ (l ranges from 0 to j with increment 1 for each term). As discussed in Sect. 2.1 here it may also be visualized that the sum in the right hand side of Eq. (7) is nothing but the sum of the coefficients arranged on a particular slanting column (depending on j) of the PT inclined to the left. This may easily be revealed from the illustration given in the Scheme 2a.

Thus for all the coefficients except the last one may be expressed as

$$\begin{aligned} a_{2j}^{(N')} = {} & k_1^2 a_{2(j-1)}^{(N'-2)} + (\text{sum of the CP coefficients starting from } a_{2(j-1)}^{(N'-2)} \\ & \text{multiplied by } \left(k_2^2\right)^l \text{ on the slanting column inclined to the left of the PT;} \\ & l \text{ ranges from 0 to } j \text{ with increment 1 for each term}) \end{aligned} \tag{8}$$

$$\text{and the last coefficient will be, } a_{2j}^{(N')} = k_1^2 a_{2(j-1)}^{(N'-2)} + k_2^{(N'-1)} \tag{9}$$

With proper rearrangement of Eq. (7) one may easily arrive at the Eq. (5) given in Sect. 2.1 to express the coefficients of any of such graphs arranged in an asymmetric



Scheme 2 **a** Illustration for the generation of the CP coefficients of the alternant edge weighted graphs of linear chains having odd number of vertices. **b** Illustration for the generation of the CP coefficients (i.e., $a_4^{(13)}$ and $a_{10}^{(13)}$) of the alternant edge weighted graphs of linear chains of odd number of vertices

PT. The use of this Eq. (5) for such graphs is illustrated in the Scheme 2b for the generation of the two coefficients, $a_4^{(13)}$ and $a_{10}^{(13)}$.

3 Characteristic polynomials of linear poly (p-phenylene) and methylene substituted linear poly (p-phenylene) graphs

Polyphenylene and its derivatives are considered to be promising candidates for low cost and easy processing materials for electro-optical and electronic applications. On account of such importance these materials have been being the focus of experimental as well as theoretical studies [19–25]. In this section above algorithms for alternant edge weighted graphs of linear chains have been utilized to find out the CP coefficients of the graphs of linear poly (p-phenylene) and methylene substituted linear poly (p-phenylene).

Let us consider a graph (G) of linear poly (p-phenylene) or methylene substituted linear poly (p-phenylene) containing N_r number of phenyl rings; G may be any one of the graphs G_3, G_4 or G_5 shown in Fig. 2. On symmetry plane factorization [26–28] the graph G is converted into a graph (G_+) of alternant edge weighted linear chain of $N(= 4N_r$ for G_3, $= 4N_r + 1$ for G_4 and $= 4N_r + 2$ for $G_5)$ number of vertices and a graph (G_-) of N_r number of graphs of ethylene molecule. As the CP of each ethylene

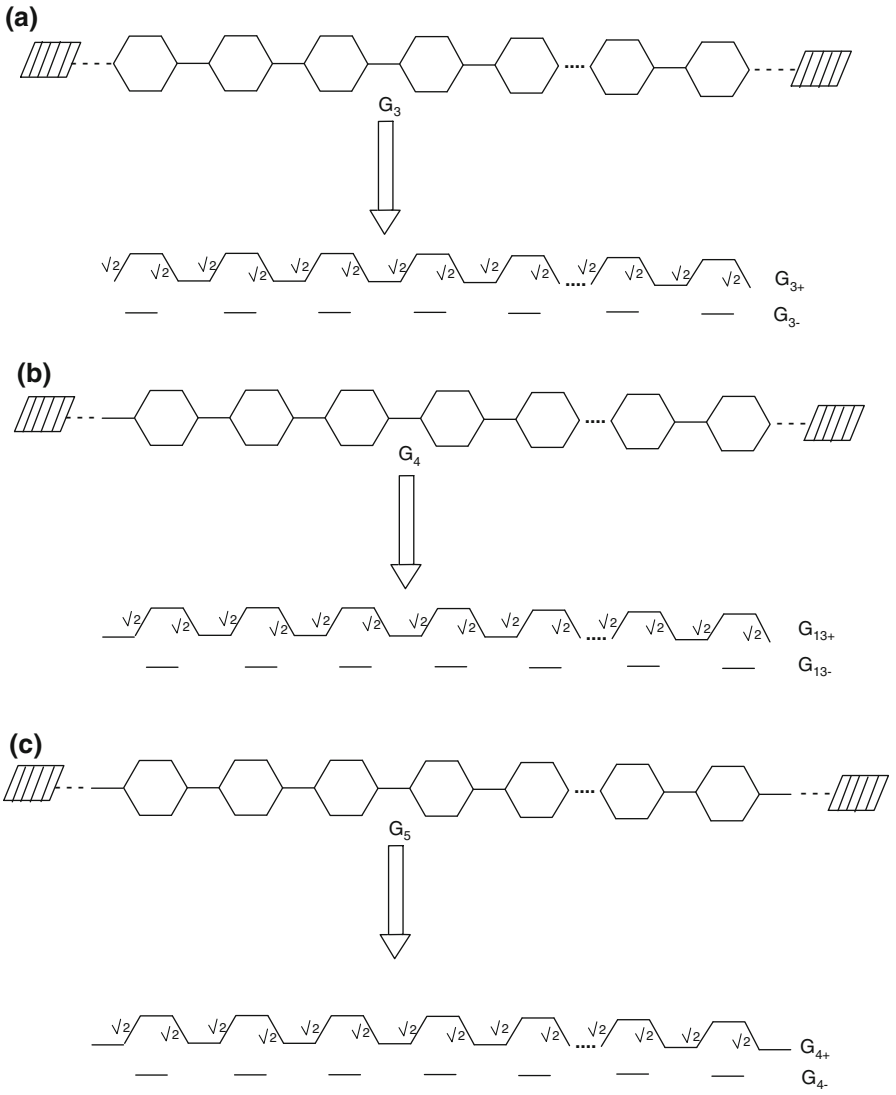


Fig. 2 Schematic mirror plane fragmentation of **a** linear poly (*p*-phenylene), **b** 1-methylene substituted linear poly (*p*-phenylene) and **c** 1,1'-dimethylene substituted linear poly (*p*-phenylene)

molecule is (x^2-1) thus the CP of G_- is $(x^2-1)^{N_r}$ whose coefficients appear as the elements of the PT and can be expressed analytically; say the $2j$th coefficient can be written as N_rC_j; where $N_rC_j = N_r!/j!(N_r-j)!$. The Let the CP of G_+ is $P(G_+,x)$. Thus the CP of the graph G will be, $P(G,x) = P(G_+,x) \times (x^2-1)^{N_r} = P(G_+,x) \times \sum_{j=0}^{N_r} [(-1)^j][{}^{N_r}C_j]x^{2N_r-2j}$ with the coefficients

$$a_{2j}^{(N+2N_r)} = \sum_{l=0}^{2N_r} {}^{N_r}C_l a_{2j-2l}^{(N)} \tag{10}$$

where $a_{2j-2l}^{(N)}$ is the $2(j-l)$th CP coefficient of the graph of alternant edge weighted linear chain of N vertices. The Eq. (10) can be written in a convenient form as a product of two matrices

$$a_{2j}^{(N+2N_r)} = \mathbf{C}^{(\mathbf{N_r})} \times (\mathbf{a}^{(\mathbf{N})})^T \tag{11}$$

where $\mathbf{C}^{(\mathbf{N_r})}$ is a row matrix, $\mathbf{C}^{(\mathbf{N_r})} = ({}^{N_r}C_0\, {}^{N_r}C_1\, {}^{N_r}C_2 \ldots {}^{N_r}C_{N_r})$ and $\mathbf{a}^{(\mathbf{N})}$ is another row matrix, $\mathbf{a}^{(\mathbf{N})} = (a_{2j}^{(N)} a_{2j-2}^{(N)} a_{2j-4}^{(N)} \ldots a_{2j-2N_r}^{(N)})$. The matrix $(\mathbf{a}^{(\mathbf{N})})^T$ is a column matrix and is the transpose of $\mathbf{a}^{(\mathbf{N})}$.

3.1 Graphs of linear poly (p-phenylene)

Linear poly (p-phenylene) compounds are important polycyclic aromatic hydrocarbons. These molecules are represented by the graph G_3 as shown in Fig. 2. The symmetry plane fragmentation [26–28] of G_3 (shown in Fig. 2) results G_{3+} and G_{3-}; G_{3+} is an alternant edge weighted ($\sqrt{2}$,1) graph of linear chain of even number of vertices with starting and ending edges of weight $\sqrt{2}$ whereas G_{3-} consists the graphs of ethylene whose number is equal to the number of benzene rings present in the graph G_3. The CP coefficients of the graph G_{3+} can be calculated with the use of Eq. (3) putting $k_1^2 = 2$ and $k_2^2 = 1$. For such graph the Eq. (4) is reduced to

$$a_{2j}^{(N')} = 2a_{2(j-1)}^{(N'-2)} + (\text{Sum of the CP coefficients starting from } a_{2(j-1)}^{(N'-2)} \text{ on the slanting column of the PT inclined to the left}) \tag{12}$$

whereas Eq. (5) is to

$$a_{2j}^{(N)} = 3a_{2(j-1)}^{(N-2)} + a_{2j}^{(N-2)} - 2a_{2(j-2)}^{(N-4)} \tag{13}$$

The asymmetric PT approach may conveniently be used with the help of either Eq. (12) or Eq. (13) to generate the coefficients of such graphs and is being illustrated in the Scheme 3.

The factorization [26–28] of a graph (G_3) of poly (p-phenylene) molecule containing N_r number of hexagonal rings shown in Fig. 2a results a graph (G_{3+}) of alternant edge weighted ($\sqrt{2}$, 1) linear chain of $N(=4N_r)$ number of vertices and a graph (G_{3-}) containing N_r number of graphs of ethylene molecule. The CP, $P(G_{3+}; x)$, of G_{3+} is obtained from the Scheme 3. Thus the CP of a linear poly (p-phenylene), $P(G_3; x)$, containing N_r number of hexagonal rings can be obtained through multiplication of $P(G_{3+}; x)$ with $(x-1)^{N_r}$. Let us illustrate the calculation of CP of biphenyl (graph G_7) shown in Fig. 3b. Symmetry plane fragmentation [26–28] of biphenyl results two graphs, G_{7+} and G_{7-}. Since G_{7-} contains two graphs of ethylene, the CP of G_{7-} is

1
1 2
1 5 4
1 8 17 8
1 11 39 49 16
1 14 70 150 129 32
1 17 110 338 501 321 64
1 20 159 640 1375 1524 769 128
1 23 217 1083 3075 4973 4339 1793 256

Scheme 3 Generation of the CP coefficients of the graphs of even vertex linear chains with alternant edge weights ($\sqrt{2}$, 1)

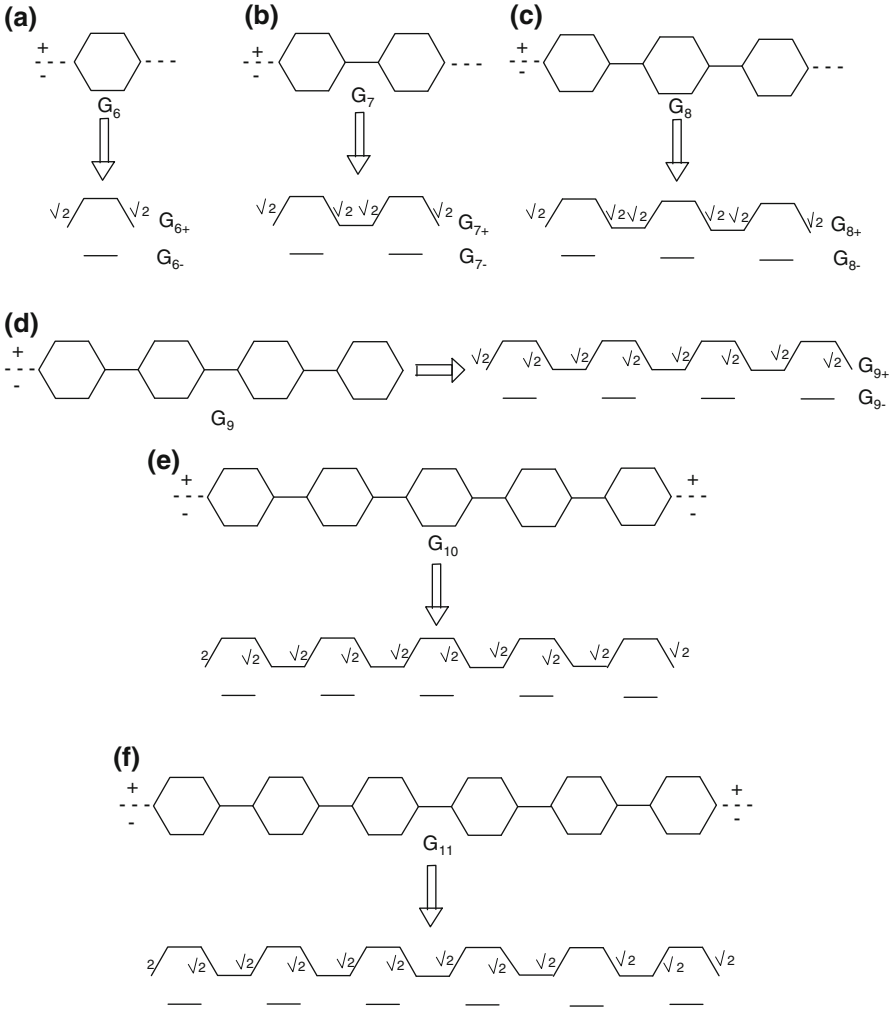


Fig. 3 Some molecular graphs of **a** benzene, **b** biphenyl, **c** *p*-terphenyl and **d** *p*-quaterphenyl along with respective symmetry plane fragments

$(x^2-1)^2$. The CP of the graph G_{7+} with 8-vertices can be obtained from the Scheme 3 and the coefficients are found to be

$$a_0^{(8)} = 1; a_2^{(8)} = 11; a_4^{(8)} = 39; a_6^{(8)} = 49; a_8^{(8)} = 16 \tag{14}$$

With the help of Eq. (11) the CP coefficients of the graph G_7 can be expressed as

$$a_{2j}^{(12)} = ({}^2C_0\ {}^2C_1\ {}^2C_2) \times \left(a_{2j}^{(8)}\ a_{2j-2}^{(8)}\ a_{2j-4}^{(8)}\right)^T = (1\ 2\ 1) \times \left(a_{2j}^{(8)}\ a_{2j-2}^{(8)}\ a_{2j-4}^{(8)}\right)^T \tag{15}$$

Thus putting $j = 0, 1, 2, \ldots, 6$ in the Eq. (15) and taking the values of the CP coefficients of the corresponding linear chain from Eq. (14) we obtain the CP coefficients of biphenyl (graph G_7) as

$$\begin{aligned}
a_0^{(12)} &= (1\ 2\ 1) \times \left(a_0^{(8)}\ a_{-2}^{(8)}\ a_{-4}^{(8)}\right)^T = (1\ 2\ 1) \times \left(1\ 0\ 0\right)^T = 1\\
a_2^{(12)} &= (1\ 2\ 1) \times \left(a_2^{(8)}\ a_0^{(8)}\ a_{-2}^{(8)}\right)^T = (1\ 2\ 1) \times \left(11\ 1\ 0\right)^T = 13\\
a_4^{(12)} &= (1\ 2\ 1) \times \left(a_4^{(8)}\ a_2^{(8)}\ a_0^{(8)}\right)^T = (1\ 2\ 1) \times \left(39\ 11\ 1\right)^T = 62\\
a_6^{(12)} &= (1\ 2\ 1) \times \left(a_6^{(8)}\ a_4^{(8)}\ a_2^{(8)}\right)^T = (1\ 2\ 1) \times \left(49\ 39\ 11\right)^T = 138\\
a_8^{(12)} &= (1\ 2\ 1) \times \left(a_8^{(8)}\ a_6^{(8)}\ a_4^{(8)}\right)^T = (1\ 2\ 1) \times \left(16\ 49\ 39\right)^T = 153\\
a_{10}^{(12)} &= (1\ 2\ 1) \times \left(a_{10}^{(8)}\ a_8^{(8)}\ a_6^{(8)}\right)^T = (1\ 2\ 1) \times \left(0\ 16\ 49\right)^T = 81\\
a_{12}^{(12)} &= (1\ 2\ 1) \times \left(a_{12}^{(8)}\ a_{10}^{(8)}\ a_8^{(8)}\right)^T = (1\ 2\ 1) \times \left(0\ 0\ 16\right)^T = 16
\end{aligned}$$

Thus the characteristic polynomial of biphenyl graph is

$$x^{12} - 13x^{10} + 62x^8 - 138x^6 + 153x^4 - 81x^2 + 16.$$

The characteristic polynomials of benzene (G_6) and some of the lower member graphs of linear poly (p-phenylene) such as p-terphenyl (G_8), p-quaterphenyl (G_9), p-quinquephenyl (G_{10}) and p-sexiphenyl (G_{11}), shown in Fig. 3, have been calculated with this procedure and are given in Table 1.

3.2 Graphs of 1-methylene substituted linear poly (p-phenylene)

The graph G_4 shown in Fig. 2b represents 1-methylene substituted linear poly (p-phenylene) containing N_r number of hexagonal rings. Symmetry plane factorization [26–28] of the graph G_4 results two graphs; G_{4+} is an alternant edge weighted $(1, \sqrt{2})$ graph of linear chain of odd number of vertices with starting edge of weight 1 and ending edge of weight $\sqrt{2}$ and the graph G_{4-} is a graph containing N_r number

Table 1 Characteristic polynomials of some graphs such as G_5, G_7, G_8, G_9, G_{10}, G_{11}, G_{12}, G_{14}, G_{15}, G_{16}, G_{18} and G_{19}

Graph	Characteristic polynomial
G_6	$x^6 - 6x^4 + 9x^2 - 4$
G_8	$x^{18} - 20x^{16} + 164x^{14} - 720x^{12} + 1862x^{10} - 2948x^8 + 2868x^6 - 1656x^4 + 513x^2 - 64$
G_9	$x^{24} - 27x^{22} + 315x^{20} - 2093x^{18} + 8802x^{16} - 24662x^{14} + 47230x^{12} - 62370x^{10} + 56429x^8 - 34111x^6 + 13047x^4 - 2817x^2 + 256$
G_{10}	$x^{30} - 34x^{28} + 515x^{26} - 4600x^{24} + 27049x^{22} - 110786x^{20} + 326331x^{18} - 704000x^{16} + 1121995x^{14} - 1321766x^{12} + 1141889x^{10} - 710152x^8 + 307275x^6 - 87030x^4 + 14337x^2 - 1024$
G_{11}	$x^{36} - 41x^{34} + 764x^{32} - 8584x^{30} + 65080x^{28} - 353188x^{26} + 1420892x^{24} - 4331208x^{22} + 10140354x^{20} - 18373950x^{18} + 25834772x^{16} - 28126808x^{14} + 23534352x^{12} - 14921716x^{10} + 7003540x^8 - 2343000x^6 + 524277x^4 - 69633x^2 + 4096$
G_{12}	$x^7 - 7x^5 + 13x^3 - 7x$
G_{14}	$x^{19} - 21x^{17} + 182x^{15} - 850x^{13} + 2352x^{11} - 4004x^9 + 4210x^7 - 2646x^5 + 903x^3 - 127x$
G_{15}	$x^{25} - 28x^{23} + 340x^{21} - 2360x^{19} + 10405x^{17} - 30664x^{15} + 61952x^{13} - 86560x^{11} + 83132x^9 - 53567x^7 + 21967x^5 - 5129x^3 + 511x$
G_{16}	$x^8 - 8x^6 + 18x^4 - 12x^2 + 1$
G_{18}	$x^{20} - 22x^{18} + 201x^{16} - 996x^{14} + 2942x^{12} - 5376x^{10} + 6012x^8 - 4172x^6 + 1569x^4 - 250x^2 + 1$
G_{19}	$x^{26} - 29x^{24} + 366x^{22} - 2650x^{20} + 12231x^{18} - 37863x^{16} + 80612x^{14} - 119068x^{12} + 121311x^{10} - 83291x^8 + 36622x^6 - 9258x^4 + 1017x^2 - 1$

of graphs of isolated ethylene molecules. In case of graph G_{4+} the Eqs. (8) and (9) are reduced to following Eqs. (16) and (17) respectively.

$$a_{2j}^{(N')} = a_{2(j-1)}^{(N'-2)} + (\text{the sum of the CP coefficients starting from } a_{2(j-1)}^{(N'-2)} \text{ multiplied by } 2^l \text{ on the slanting column inclined left of the PT; } l \text{ ranges from 0 to } j \text{ with increment 1 for each term}) \tag{16}$$

and the last coefficient is obtained as

$$a_{2j}^{(N')} = a_{2(j-1)}^{(N'-2)} + 2^{(N'-1)/2} \tag{17}$$

These equations are conveniently used to obtain the CP coefficients of such graphs. Again for such graphs the Eq. (5) is reduced to Eq. (13) as given in Sect. 3.1.

Using either the Eqs. (16) and (17) or the Eq. (13), the CP coefficients of the graph G_{4+} has been generated and is illustrated in an asymmetric PT array as been shown in the Scheme 4.

Now the characteristic polynomial of the graph (G_4) of 1-methylene substituted linear poly (p-phenylene) can be obtained by the multiplication the CP of the graph G_{4+} with that of G_{4-}. This multiplication may easily be done with the help of Eq. (10) as discussed in the cases of linear poly (p-phenylene) in the Sect. 3.1. This procedure is illustrated with the graph of 1-methylene substituted linear biphenyl (G_{13}) shown in Fig. 4b. Factorization of G_{13} with the help of the plane of symmetry [26–28] results

1
1 3
1 6 7
1 9 23 15
1 12 48 72 31
1 15 82 198 201 63
1 18 125 420 699 522 127
1 21 177 765 1795 2223 1291 255
1 24 238 1260 3840 6768 6562 3084 511

Scheme 4 Generation of the CP coefficients of the graphs of odd vertex linear chain with alternant edge weights $(1, \sqrt{2})$

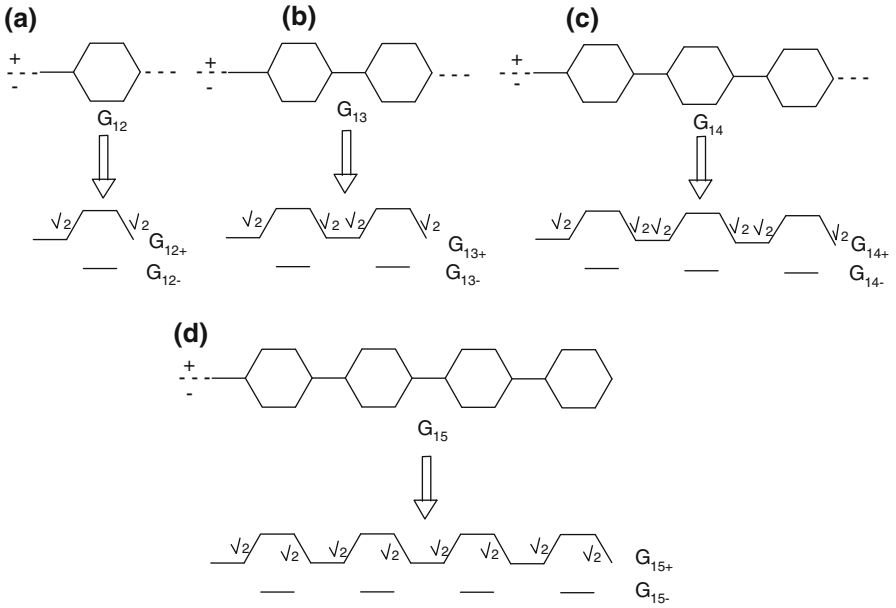


Fig. 4 Some molecular graphs of **a** 1-methylene benzene, **b** 1-methylene biphenyl, **c** 1-methylene terphenyl and **d** 1-methylene quaterphenyl

two graphs, G_{13+} and G_{13-} as given in Fig. 4b. The CP of the graph G_{13+}, which is an alternant edge weighted graphs of linear chain of 9 vertices, has been obtained from the PT given in the Scheme 4 and its coefficients are found to be

$$a_0^{(9)} = 1; a_2^{(9)} = 12; a_4^{(9)} = 48; a_6^{(9)} = 72; a_8^{(9)} = 31 \tag{18}$$

Again the CP of the graph G_{13-} containing two ethylene graphs will be $(x^2 - 1)^2$. The CP of the graph G_{13} may easily be expressed with the help of Eq. (11) as

$$a_{2j}^{(13)} = ({}^2C_0\ {}^2C_1\ {}^2C_2) \times \left(a_{2j}^{(9)}\ a_{2j-2}^{(9)}\ a_{2j-4}^{(9)}\right)^T = (1\ 2\ 1) \times \left(a_{2j}^{(9)}\ a_{2j-2}^{(9)}\ a_{2j-4}^{(9)}\right)^T \tag{19}$$

with the use of Eqs. (18) and (19) we may easily obtain the CP coefficients of the graph G_{13} as

$$\begin{aligned}
a_0^{(13)} &= (1\ 2\ 1) \times \left(a_0^{(9)}\ a_{-2}^{(9)}\ a_{-4}^{(9)}\right)^T = (1\ 2\ 1) \times (1\ 0\ 0)^T = 1\\
a_2^{(13)} &= (1\ 2\ 1) \times \left(a_2^{(9)}\ a_0^{(9)}\ a_{-2}^{(9)}\right)^T = (1\ 2\ 1) \times (12\ 1\ 0)^T = 14\\
a_4^{(13)} &= (1\ 2\ 1) \times \left(a_4^{(9)}\ a_2^{(9)}\ a_0^{(9)}\right)^T = (1\ 2\ 1) \times (48\ 12\ 1)^T = 73\\
a_6^{(13)} &= (1\ 2\ 1) \times \left(a_6^{(9)}\ a_4^{(9)}\ a_2^{(9)}\right)^T = (1\ 2\ 1) \times (72\ 48\ 12)^T = 180\\
a_8^{(13)} &= (1\ 2\ 1) \times \left(a_8^{(9)}\ a_6^{(9)}\ a_4^{(9)}\right)^T = (1\ 2\ 1) \times (31\ 72\ 48)^T = 223\\
a_{10}^{(13)} &= (1\ 2\ 1) \times \left(a_{10}^{(9)}\ a_8^{(9)}\ a_6^{(9)}\right)^T = (1\ 2\ 1) \times (0\ 31\ 72)^T = 134\\
a_{12}^{(13)} &= (1\ 2\ 1) \times \left(a_{12}^{(9)}\ a_{10}^{(9)}\ a_8^{(9)}\right)^T = (1\ 2\ 1) \times (0\ 0\ 31)^T = 31
\end{aligned}$$

So the CP of 1-methylene biphenyl (G_{13}) is

$$x^{13} - 14x^{11} + 73x^9 - 180x^7 + 223x^5 - 134x^3 + 31x.$$

The characteristic polynomials of 1-methylene benzene (G_{12}) and some of the lower member graphs of this series such as 1-methylene substituted p-terphenyl (G_{14}) and 1-methylene substituted quaterphenyl (G_{15}) shown in Fig. 4 have been calculated with this procedure and the characteristic polynomials are given in Table 1.

3.3 Graphs of 1, 1'-dimethylene substituted linear poly (p-phenylene)

The graph G_5, shown in Fig. 2c can be used to represent 1, 1'-dimethylene substituted linear poly (p-phenylene) molecules. The symmetry plane fragmentation [26–28] of G_5 (shown in Fig. 2c) results G_{5+} and G_{5-}; G_{5+} is an alternant edge weighted $(1, \sqrt{2})$ graph of linear chain of even number of vertices with starting and ending edges of weight 1 whereas G_{5-} consists the graphs of ethylene whose number is equal to the number of hexagonal rings present in the graph G_5. The CP coefficients of the graph G_{5+} can be calculated with the use of Eq. (3) putting $k_1^2 = 1$ and $k_2^2 = 2$. For this graph the Eq. (4) is reduced to

$$a_{2j}^{(N')} = a_{2(j-1)}^{(N'-2)} + (\text{sum of the CP coefficients starting from the element } a_{2(j-1)}^{(N'-2)} \text{ multiplied by } 2^l \text{ on the slanting column inclined to the left ofthe PT; } l \text{ ranges from 0 to } j \text{ with increment 1 for each term}) \tag{20}$$

1
1 1
1 4 1
1 7 11 1
1 10 30 26 1
1 13 58 102 57 1
1 16 95 256 303 120 1
1 19 141 515 955 825 247 1
1 22 196 906 2310 3178 2116 502 1

Scheme 5 Generation of the CP coefficients of the graphs of even vertex linear chain with alternant edge weights $(1, \sqrt{2})$

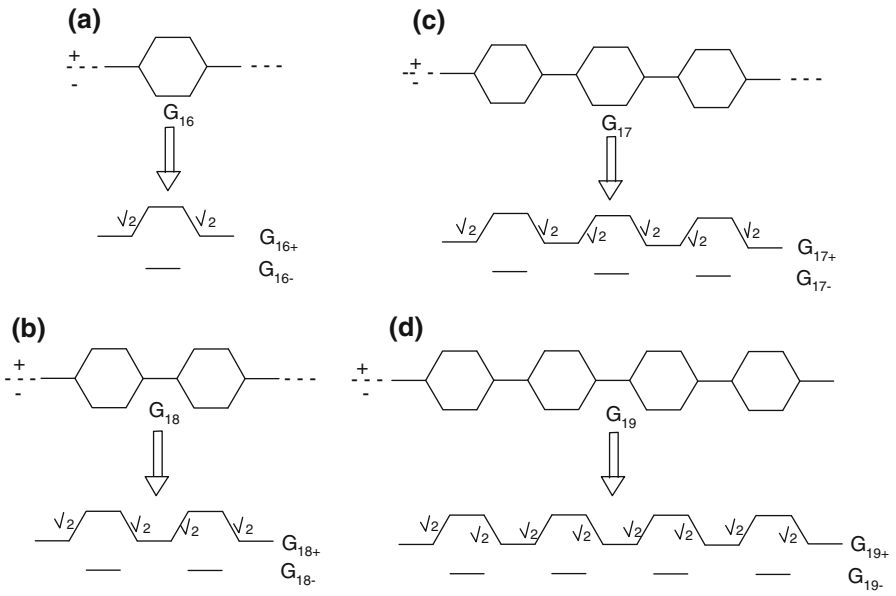


Fig. 5 Some molecular graphs of **a** *p*-dimethylene benzene, **b** 1,1'-dimethylene biphenyl, **c** 1,1'-dimethylene terphenyl, and **d** 1,1'- dimethylene quaterphenyl along with respective symmetry plane fragments

whereas Eq. (5) is reduced to the Eq. (13) as shown in the earlier Sect. 3.1.

Generation of the CP coefficients of the graph G_{5+} with the use of the asymmetric PT approach guided by the Eq. (20) has been illustrated in the Scheme 5.

On symmetry plane factorization [26–28] the 1,1'-dimethylene substituted linear poly (*p*-phenylene) graph represented by G_5 is converted into the graph G_{5+} of $(4N_r + 2)$ vertices and the graph G_{5-} of N_r number of graphs of ethylene molecule as shown in Fig. 2c. Thus the multiplication of the CP of G_{5+} and that of G_{5-} results the CP of the graph G_5 and this can easily be achieved with the use of Eq. (11). Let us illustrate this procedure with graph of *p*-dimethylene substituted biphenyl (G_{17}) shown in Fig. 5b. The CP of the graph G_{17+} of 10 vertices obtained from symmetry plane fragmentation [26–28] of G_{17}, shown in the Fig. 5b, can be easily calculated from the Scheme 5 and its coefficients are found to be

$$a_0^{(10)} = 1; a_2^{(10)} = 13; a_4^{(10)} = 58; a_6^{(10)} = 102; a_8^{(10)} = 57; a_{10}^{(10)} = 1. \quad (21)$$

The CP of the graph G_{17-} containing two ethylene graphs will be $(x^2-1)^2$. Thus with the use of Eq. (11) the CP coefficients of the G_{17} can be expressed as

$$a_{2j}^{(14)} = ({}^2C_0\ {}^2C_1\ {}^2C_2) \times \left(a_{2j}^{(10)}\ a_{2j-2}^{(10)}\ a_{2j-4}^{(10)}\right)^T = (1\ 2\ 1) \times \left(a_{2j}^{(10)}\ a_{2j-2}^{(10)}\ a_{2j-4}^{(10)}\right)^T \quad (22)$$

Combining the Eqs. (21) and (22) we may evaluate the CP coefficients of the graph G_{17} as

$$a_0^{(14)} = (1\ 2\ 1) \times \left(a_0^{(10)}\ a_{-2}^{(10)}\ a_{-4}^{(10)}\right)^T = (1\ 2\ 1) \times \left(1\ 0\ 0\right)^T = 1$$

$$a_2^{(14)} = (1\ 2\ 1) \times \left(a_2^{(10)}\ a_0^{(10)}\ a_{-2}^{(10)}\right)^T = (1\ 2\ 1) \times \left(13\ 1\ 0\right)^T = 15$$

$$a_4^{(14)} = (1\ 2\ 1) \times \left(a_4^{(10)}\ a_2^{(10)}\ a_0^{(10)}\right)^T = (1\ 2\ 1) \times \left(58\ 13\ 1\right)^T = 85$$

$$a_6^{(14)} = (1\ 2\ 1) \times \left(a_6^{(10)}\ a_4^{(10)}\ a_2^{(10)}\right)^T = (1\ 2\ 1) \times \left(102\ 58\ 13\right)^T = 231$$

$$a_8^{(14)} = (1\ 2\ 1) \times \left(a_8^{(10)}\ a_6^{(10)}\ a_4^{(10)}\right)^T = (1\ 2\ 1) \times \left(57\ 102\ 58\right)^T = 319$$

$$a_{10}^{(14)} = (1\ 2\ 1) \times \left(a_{10}^{(10)}\ a_8^{(10)}\ a_6^{(10)}\right)^T = (1\ 2\ 1) \times \left(1\ 57\ 102\right)^T = 217$$

$$a_{12}^{(14)} = (1\ 2\ 1) \times \left(a_{12}^{(10)}\ a_{10}^{(10)}\ a_8^{(10)}\right)^T = (1\ 2\ 1) \times \left(0\ 1\ 57\right)^T = 59$$

$$a_{14}^{(14)} = (1\ 2\ 1) \times \left(a_{14}^{(10)}\ a_{12}^{(10)}\ a_{10}^{(10)}\right)^T = (1\ 2\ 1) \times \left(0\ 0\ 1\right)^T = 1$$

So the characteristic polynomials of *p*-dimethylene substituted biphenyl (G_{17}) will be

$$x^{14} - 15x^{12} + 85x^{10} - 231x^8 + 319x^6 - 217x^4 + 59x^2 - 1$$

The characteristic polynomials of *p*-dimethylene benzene (G_{16}) and some of the lower member graphs of 1, 1'-dimethylene substituted linear poly (*p*-phenylene) such as 1,1'-dimethylene substituted *p*-terphenyl (G_{18}) and 1,1'-dimethylene substituted quaterphenyl (G_{19}) shown in Fig. 5 have been calculated with this procedure and are given in Table 1.

4 Sum of characteristic polynomial coefficients ($S_{\mathrm{CP}}^{N_r}$)

Since CP of any graph is a graph invariant, the sum of characteristic polynomial coefficients ($S_{\mathrm{CP}}^{N_r}$) of a graph can be used as topological index (analogous to the Hosoya index [29] which is the sum of the matching polynomial coefficients) to

predict physicochemical properties of molecules represented by such graphs. $S_{\mathrm{CP}}^{N_r}$ of a poly (p-phenylene) graph can directly be calculated by summing up the CP coefficients of the respective graph but this type of calculation become much cumbersome as the number of rings increases. Thus for such calculations it is convenient to express $S_{\mathrm{CP}}^{N_r}$ of a poly (p-phenylene) graph in terms of the sums of the CP coefficients of the preceding poly (p-phenylene) graphs of its lower analogs. The desired expression can easily be derived using Eqs. (10) and (13) and is as follows.

Taking sum over j (j ranges from 0 to n; $n = (N + 2N_r)/2$ for linear poly (p-phenylene), $n = (N - 1 + 2N_r)/2$ for 1-methylene substituted linear poly (p-phenylene) and $n = (N + 2 + 2N_r)/2$ for 1, 1'-dimethylene substituted linear poly (p-phenylene)) on both sides of Eq. (13) of an alternant edge weighted linear chain with N number of vertices we have

$$\begin{aligned}\sum_{j=o}^{n} a_{2j}^{(N)} &= 3\sum_{j=o}^{n} a_{2(j-1)}^{(N-2)} + \sum_{j=o}^{n} a_{2j}^{(N-2)} - 2\sum_{j=o}^{n} a_{2(j-2)}^{(N-4)} = 4\sum_{j=o}^{n} a_{2j}^{(N-2)} - 2\sum_{j=o}^{n} a_{2j}^{(N-4)} \\ &= 16\sum_{j=o}^{n} a_{2j}^{(N-4)} - 8\sum_{j=o}^{n} a_{2j}^{(N-6)} - 2\sum_{j=o}^{n} a_{2j}^{(N-4)} \\ &= 12\sum_{j=o}^{n} a_{2j}^{(N-4)} - 4\sum_{j=o}^{n} a_{2j}^{(N-8)} \end{aligned} \tag{23}$$

Now the sum of the CP coefficients ($S_{\mathrm{CP}}^{N_r}$) of any one of these three types of linear poly (p-phenylene) graphs containing N_r number of hexagonal ring can be written with the help of Eq. (10) as

$$S_{\mathrm{CP}}^{N_r} = \sum_{j=0}^{n} a_{2j}^{(N+2N_r)} = \sum_{j=0}^{n}\sum_{l=0}^{N_r} {}^{N_r}C_l a_{2j-2l}^{(N)} \tag{24}$$

Introducing Eq. (23) into the Eq. (24) we may obtain

$$\begin{aligned} S_{\mathrm{CP}}^{N_r} &= \sum_{j=0}^{n} a_{2j}^{(N+2N_r)} = 12\sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r}C_l a_{2j-2l}^{(N-4)} - 4\sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r}C_l a_{2j-2l}^{(N-8)} \\ &= 12\left[\sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r-1}C_l a_{2j-2l}^{(N-4)} + \sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r-1}C_l a_{2j-2-2l}^{(N-4)}\right] \\ &\quad -4\left[\sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r-1}C_l a_{2j-2l}^{(N-8)} + \sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r-1}C_l a_{2j-2-2l}^{(N-8)}\right] \\ &= 24\sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r-1}C_l a_{2j-2l}^{(N-4)} - 8\sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r-1}C_l a_{2j-2l}^{(N-8)} \end{aligned}$$

Table 2 The values of the sum of CP coefficients ($S_{CP}^{N_r}$) of linear poly (p-phenylene) (PPP), 1-methylene substituted linear PPP and 1, 1'-dimethylene substituted linear PPP containing 1-6 phenyl rings calculated with the use of Eq.(25)

Linear PPP		1-methylene substituted linear PPP		1, 1'-dimethylene substituted linear PPP	
Number of ring (N_r)	Sum of CP coefficients ($S_{CP}^{N_r}$)	Number of ring (N_r)	Sum of CP coefficients ($S_{CP}^{N_r}$)	Number of ring (N_r)	Sum of CP coefficients ($S_{CP}^{N_r}$)
1	20	1	28	1	40
2	464	2	656	2	928
3	10816	3	15296	3	21632
4	252160	4	356608	4	504320
5	5878784	5	8313856	5	11757712
6	137056256	6	193826816	6	274115968

$$= 24S_{CP}^{N_r-1} - 8\left[\sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r-2}C_l a_{2j-2l}^{(N-8)} + \sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r-2}C_l a_{2j-2-2l}^{(N-8)}\right]$$

$$= 24S_{CP}^{N_r-1} - 16\sum_{l=0}^{N_r}\sum_{j=0}^{n} {}^{N_r-2}C_l a_{2j-2l}^{(N-8)} = 24S_{CP}^{N_r-1} - 16S_{CP}^{N_r-2}. \quad (25)$$

The Eq. (25) is a recurrence relation and is useful to calculate the values of $S_{CP}^{N_r}$ for any such linear poly (p-phenylene) graphs from the knowledge of the values of the sum of the CP coefficients of two successive members of its lower analogs obtained from their corresponding CPs. The values of $S_{CP}^{N_r}$ for few such graphs have been calculated with the help of Eq. (25) and are given in Table 2.

Recently ambient conditions density (ρ_0) and the bulk modulus (β) of poly (p-phenylene) containing two to six phenyl rings have been reported [21]. Very recently a good linear correlation of ambient conditions density and bulk modulus of poly (p-phenylene) containing two to six hexagonal rings with the $W^{1/4}$ (W is the Weiner index) has been established [30]. Here we have investigated the variation of ρ_0 and β with the sum of CP coefficients ($S_{CP}^{N_r}$). The values of ambient conditions density (ρ_0) and bulk modulus (β) are taken from the work of Heimel *et al.* [21] and all these values along with the values of log $S_{CP}^{N_r}$ for linear poly (p-phenylene) containing two to six phenyl rings are given in Table 3. It is found that except biphenyl the plot of ambient conditions density (ρ_0) taken from the work of Heimel *et al.* [21] vs. logarithm of the sum of the CP coefficients (log $S_{CP}^{N_r}$) bears an excellent linear relationship as shown in Fig. 6. The equation that represents such relationship is as follows.

$$\rho_0 = (0.7015 \pm 0.0083) + (0.0103 \pm 0.0013) \log S_{CP}^{N_r};\ (\text{correlation coeff.} = 0.98) \quad (26)$$

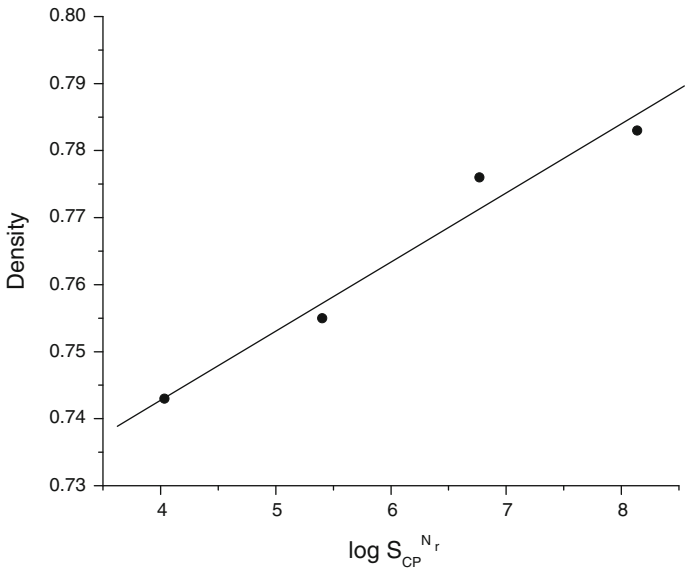


Fig. 6 Plot of ambient conditions density (ρ_0) *vs.* log S_{CP} of linear poly (p-phenylene) containing two to six phenyl rings

The plot of the bulk modulus (β) taken from the work of Heimel *et al.* [21] vs. log S_{CP} of linear poly (p-phenylene), except biphenyl which deviates from the linearity, results a good straight line as shown in Fig. 7. The equation that fits the straight line is

$$\beta = (45.172 \pm 2.974) + (6.873 \pm 0.474) \log S_{CP}^{N_r}; \text{(correlation coeff.} = 0.99) \tag{27}$$

The bulk modulus of biphenyl obtained from the above linear relationship is found to be 63.5 k bar, which is nearer to the values 54 and 59 k bar obtained for biphenyl by Vaidya *et al.* [31] and Bhadra [32] respectively compared to that of Heimel *et al.* [21].

In the work of Heimel *et al.* [21] it has been shown that the bulk properties like ambient condition density (ρ_0) and bulk modulus (β) vary linearly with the number of phenyl rings i.e., the length of poly (p-phenylene) compounds containing two to six phenyl rings. In the present study we have found that these bulk properties bear a good linear relationship with the logarithm of the sum of the CP coefficients i.e., $\log S_{CP}^{N_r}$. This may be explained as follows.

The CP coefficients are combinatorial quantities and depend on the number of vertices as well as the number of edges that connect the vertices in a graph. Thus with the increase in the number of phenyl rings in the poly (p-phenylene) systems the number of CP coefficients along with their numerical values tend to increase in a greater extent that ultimately lead large values of the sum of CP coefficients ($S_{CP}^{N_r}$). Such high values of the sum of CP coefficients ($S_{CP}^{N_r}$) with the increase in the number of phenyl rings can be assumed to be proportional to a quantity expressed in terms of number of phenyl

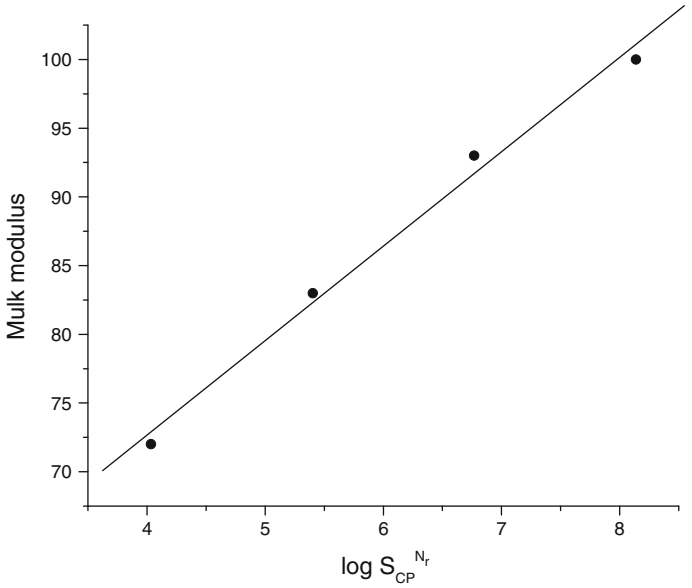


Fig. 7 Plot of bulk modulus (β) *vs.* log S_{CP} of linear poly (p-phenylene) containing three to six phenyl rings

rings raised in power. Thus the logarithm of S_{CP} should vary linearly with the number of phenyl rings. Such assumption will be better for higher the number of phenyl ring for such poly (p-phenylene) systems. Thus for biphenyl, which is the simplest in poly (p-phenylene) system the plots of ambient conditions density (ρ_0) and bulk modulus (β) vs. log $S_{CP}^{N_r}$ deviate from linearity.

5 Kekulé valence structures

The study on the Kekulé valence structures [33–35] has been the focus of long time attractions for many researchers. The number of Kekulé valence structures that a molecular graph may have is directly related to the last coefficient (i.e., the coefficient of x^0, say a_N) of the characteristic polynomial of the said graph [13,14,33]. Let K is the number of Kekulé valence structures of a molecular graph with N number of vertices, then $K = \sqrt{a_N}$. Since CP coefficients of the graphs of linear poly (p-phenylene) or methylene substituted linear poly (p-phenylene) are generated from the CP coefficients of their respective right hand (+) mirror fragments, the last coefficients of the CPs of the graphs of linear poly (p-phenylene) or methylene substituted linear poly (p-phenylene) will be same with that of their respective right hand (+) mirror fragments. The number of Kekulé valence structures of linear poly (p-phenylene) can be obtained from Scheme 3 and is found to be 2^{N_r} (N_r is the number of hexagonal rings). The values of K for biphenyl, p-terphenyl, p-quaterphenyl and p-quinquephenyl and p-sexiphenyl are given in Table 3. From the Scheme 4 the number of Kekulé valence structures of 1-methylene linear poly (p-phenylene) is found to be $K = 0$ for

Table 3 Logarithms of the sum of CP coefficients (log $S_{CP}^{N_r}$) and the Kekulé valence structures count (log K) of linear poly (*p*-phenylene) (PPP) along with the ambient conditions density and bulk modulus of the molecules of linear PPP with two to six phenyl rings

Linear PPP	log $S_{CP}^{N_r}$	Kekulé valence structures count (K)	log K	Density (ρ_0) (amu Å^{-3})	Bulk modulus (β) (k bar)
G_7	2.667	4	0.602	0.713	43
G_8	4.034	8	0.903	0.743	72
G_9	5.402	16	1.204	0.755	83
G_{10}	6.769	32	1.503	0.776	93
G_{11}	8.137	64	1.806	0.783	100

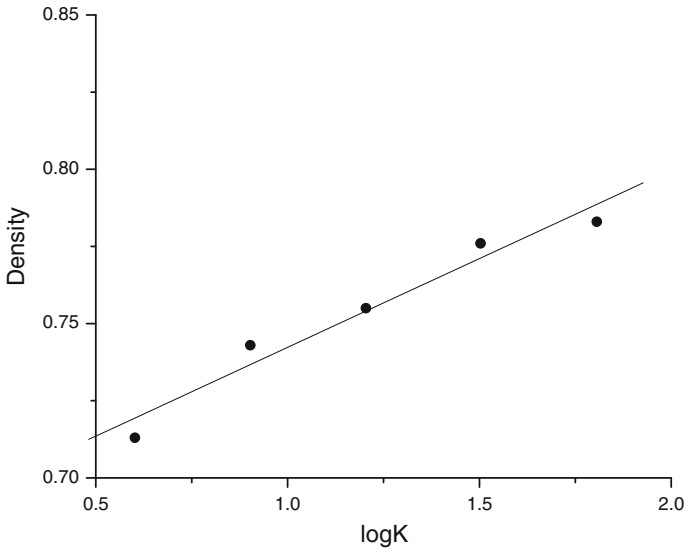


Fig. 8 Plot of ambient conditions density (ρ_0) *vs.* log K of linear poly (*p*-phenylene) containing two to six phenyl rings

all value of N_r. Again from the Scheme 5 we can see that in case of 1, 1' dimethylene substituted linear poly (*p*-phenylene), $K = 1$ for all value of N_r.

Kekulé valence structures are important parameter to characteristic polycyclic conjugated hydrocarbon, to calculate molecular resonance energy, to predict aromaticity, to guess the reactivity, to assess the stability etc. of polycyclic aromatic hydrocarbons [33–35]. In this article we have searched the variation of ambient conditions density (ρ_0) and the bulk modulus (β) of linear poly (*p*-phenylene) containing two to six phenyl rings with their respective Kekulé valence structures count (K). All the values of ρ_0, $\beta$and K are given in Table 3. The plot of ρ_0 vs. log K is a good straight line as shown in Fig. (8) and it complies with the following equation

$$\rho_0 = (0.685 \pm 0.009) + (0.0575 \pm 0.007) \log K; \text{(correlation coeff.} = 0.98) \quad (28)$$

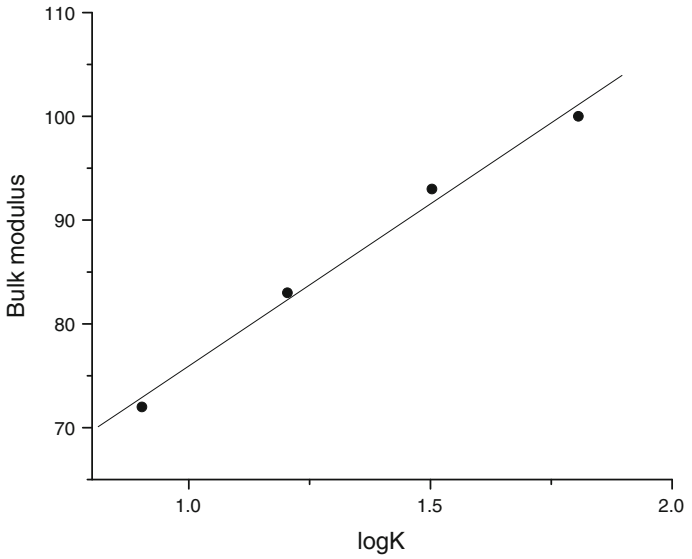


Fig. 9 Plot of bulk modulus (β) *vs.* log S_{CP} of linear poly (p-phenylene) containing three to six phenyl rings

The βvalues of all linear poly (p-phenylene) (except biphenyl that deviates from linearity), given in Table 3, bear linear relationship with their respective log K values as shown in Fig. (9). The equation that fits with this linearity is as follows.

$$\beta = (44.695 \pm 3.064) + (31.244 \pm 2.196) \log K; \text{(correlation coeff.} = 0.99) \quad (29)$$

The value of β for biphenyl calculated with the use of Eq. (26) is found to be 63.5 k bar, which is same as has been obtained from the sum of CP coefficients ($S_{CP}^{N_r}$) in Sect. 4.

6 Conclusion

The characteristic polynomials (CP) of graphs have many applications. The CP of a graph can be used to calculate eigenvalues of the molecular graph. The CPs have been used to obtain many important results [36] about total π-electron energy through the use of Coulson function [37,38] for a wide variety of graphs [13,14] ranging from small molecules to large molecules like fullerenes. Besides these characteristic polynomials have applications in chemical kinetics [39], estimating stabilities of conjugated molecules and electronic structure of organic polymer and periodic structures [13,14,40]. Very recently characteristic polynomial of sub units are used to calculate opacity polynomials of composite systems, vanishing of which dictates the zero conductance at a given energy for tight-binding source and sink potential (SSP) model of transmission in single molecule π-conjugated conductor [41]. The graphs of methylene substituted linear poly (p-phenylene) possess zero eigenvalue in their

eigenspectra as is evident from the respective CPs, so these graphs with infinite number of rings possess conduction band adjacent to its valence band and are predicted to be organic conductors [14,42]. The graphs discussed in this paper are important chemical compounds and many of these compounds have important photophysical properties [20–25]. For example, both *p*-terphenyl and *p*-quaterphenyl are used as UV laser dyes [22], in scintillation counters [23] and a wavelength shifters [22], whereas *p*-sexiphenyl is used as active component in thin film organic LEDs (OLEDs), showing polarized blue emission [25].

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