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CYCLE DECOMPOSITIONS OF LINEAR BENZENE CHAINS

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Abstract

Two linear recurrences are determined, from which circuit polynomials of linear benzene chains can be explicitly obtained. Corresponding results for characteristic polynomials, matching polynomials and μ-polynomials can be easily deduced.

Keywords and Phrases

cycle	linear benzene chain
cycle cover	characteristic polynomial
circuit polynomial	matching polynomial
proper cycles	μ-polynomial
polyacenes	

1. INTRODUCTION

We will consider only graphs which are finite and have no loops. Let G be such a graph. A cycle decomposition (circuit cover, cycle cover) of G, is a spanning subgraph of G, in which every component is a circuit. We define a circuit with one and two nodes to be a node and and edge respectively. A circuit with more than two nodes will be called a proper circuit. A matching is a circuit cover which has no proper circuits. With every circuit (cycle) α in G, let us associate an indeterminate or weight w_α and with every cycle cover C, the weight

$$w(C) = \Pi w_\alpha,$$

where the product is taken over all the cycles in C. Then the circuit (cycle) polynomial of G is

$$C(G;\underline{w}) = \sum w(C),$$

where the summation is taken over all the cycle covers in G, and $\underline{w}$ is a vector of weights, sometimes referred to as a weight vector. The circuit polynomial was first introduced in Farrell [2] as a member of a class of polynomials, called F-polynomials. The basic results about circuit polynomials are however given in Farrell [1].

In this paper, we will assign the weight w_n to the cycle with n nodes. Therefore $\underline{w}$ will be of the form $(w_1,w_2,w_3,\ldots,w_p)$, where p is the number of nodes in G.

Therefore if $Aw_i^r w_j^s w_k^t$ is a term in $C(G;\underline{w})$, then $ri + js + kt = p$ and G has A covers consisting of r i-gons, s j-gons and t k-gons. $C(G;\underline{w})$ is essentially a generating function for the different types of circuit covers of G.

We define a linear benzene chain B_n to be the graph formed by edge concatenating n(a finite number) hexagons, so that the adjacent hexagons have exactly one edge in common. This graph can also be called a hexagonal animal (see Harary and Harborth [11]). Among regular chemical structures nature seems to prefer haxagonal structures. Thus benzene chains are of particular interest to chemists. The corresponding chemical compounds are called polyacenes. ($n = 1$; benzene, $n = 2$; naphthalene $n = 3$; anthracene, etc.)

It was shown in [2] that the characteristic polynomial and the matching polynomial are special circuit polynomials. Thus, statements about $C(G;\underline{w})$ will also hold for these two polynomials. The characteristic polynomial and the matching polynomial are of some importance in the investigation of chemical compounds (see Godsil and Gutman [6,7] and Gutman [8]). Recently, another polynomial, the μ-polynomial, was introduced by Gutman and Polansky [9]. This polynomial also seems to be quite useful in chemical investigations on π-electron energy (see [9] and Polansky and Graovac [13]). It was shown by Farrell [3] that this polynomial is also a special circuit polynomial. Thus, results about circuit polynomials of benzene chains could be of interest to theoretical chemists.

We will derive two linear recurrences, from which the circuit polynomial of B_n can be explicitly obtained, for any value of n. We will also give some tables of values of $C(B_n;\underline{w})$. For brevity, we will use $C(B_n)$ (and sometimes B_n), for $C(B_n;\underline{w})$, when it would lead to no confusion, and especially in equations. We refer the reader to Harary [10] for the basic definitions in Graph Theory.

2. PRELIMINARIES

We define a chain to be a tree with nodes of valencies 1 and 2 only. The chain with n nodes will be denoted by P_n. Most of our results will be written in terms of the circuit polynomial of P_n. Clearly, every circuit cover of P_n will be a matching. Therefore the circuit polynomial of P_n coincides with its matching polynomial. Hence from Theorem 9 of Farrell [4], we have the following lemma.

Lemma 1

(i) $$C(P_p;\underline{w}) = \sum_{k=0}^{[p/2]} \binom{p-k}{k} w_1^{p-2k} w_2^{k} .$$

(ii) $$C(P_p)=w_1 C(P_{p-1}) + w_2\, C(P_{p-2}), \text{ with } C(P_0) = 1.$$

A table of values for $C(P_p)$ is also given in [4] (Table 1). This will be useful in the material which follows. We attach P_n to a graph G, by identifying an end node of P_n with a node of G.

The following result is called the Fundamental Theorem for circuit polynomials. It can be easily proved (see [1]).

Theorem 1

Let G be a graph containing an edge xy, joining nodes x and y. Then

$$C(G;\underline{w}) = C(G';\underline{w}) + w_2\, C(G'';\underline{w}) + C(G^*;\underline{w}),$$

where G' is the graph obtained from G by deleting xy, G'' is obtained from G by removing nodes x and y, and G^* is the restricted graph obtained from G, by requiring that any cover of G^* must include edge xy as part of a proper circuit.

Theorem 1 implies an algorithm for finding circuit polynomials of graphs. This algorithm will be referred to as the reduction process.

We will denote the characteristic polynomial of the graph G by $\Phi(G;x)$, its matching polynomial by $m(G;w_1,w_2)$ and its μ-polynomial by $\mu(G;\underline{t},x)$. The corresponding brief notations will be $\Phi(G)$, $m(G)$ and $\mu(G)$ respectively. The following result was established in [1,2].

Lemma 2

$\Phi(G;x)$ is obtained from $C(G;w)$ by putting $w_1 = x$, $w_2 = -1$ and $w_k = -2$, for $k>2$ i.e. by putting $\underline{w} = (x,-1,-2,-2,\ldots,-2)$.

From the definition of a matching, we have

Lemma 3

$$m(G;w_1,w_2) = C(G;(w_1, w_2, 0, 0, \ldots,0)).$$

The following lemma is taken from [3]. (Theorem 1, with the signs corrected).

Lemma 4

$$\mu(G;\underline{t},x) = C(G; (x,-1, -2t_1, -2t_2,\ldots)),$$

where $\underline{t} = (t_1,t_2,t_3,\ldots)$.

The following lemma was established in [9] and [13]; otherwise it can be easily deduced from Lemmas 2,3 and 4.

Lemma 5

(i) $\Phi(G;x)) = \mu(G;\underline{1},x)$ and

(ii) $\alpha(G;x) = \mu(G;\underline{0},x)$, where

$\alpha(G;x) = m(G; x,-1)$ is the acyclic polynomial of G.

3. CIRCUIT POLYNOMIALS OF BENZENE CHAINS

We will call the n hexagons which are "stuck on" to form B_n, the cells of B_n. We define B_0 to be an edge. The first and last cells of B_n will be called terminal cells. B_n is illustrated below in Figure 1.

B_n:

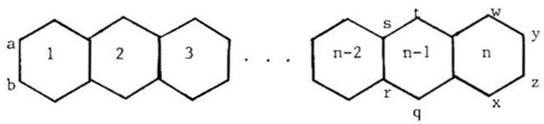
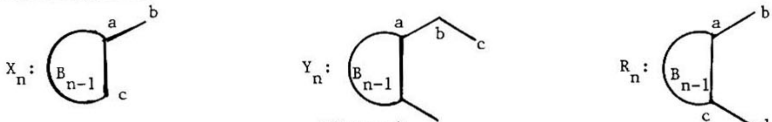


Figure 1

Edges ab and yz will be called <u>terminal</u> <u>edges</u>. Nodes a,b,y and z will be called <u>terminal</u> <u>nodes</u>.



<u>Figure 2</u>

It is clear from the diagrams that X_1, Y_1 and R_1 are the chains P_3, P_5 and P_4 respectively. We will take X_0, Y_0, and R_0 to be the empty graph.

Let us apply, the reduction process to B_n, by deleting the edge uw (see Figure 1). Then (in the notation of Theorem 1) G' will be the graph obtained from B_{n-1} by attaching P_5(vxzyw) to one of its terminal nodes, node v. G'' will be B_{n-2} with P_2 (st) and P_6(rqrxzy) attached to the nodes r and s respectively, of a terminal edge rs. G^* will be the restricted graph in which uw must be part of a proper cycle, in every cycle cover of B_n.

Apply the reduction process to the graph B_n; using edge vx, and to the subsequent graphs G' and G'', using edges which cannot belong to proper cycles. This yields (with G written for $C(G;\underline{w})$),

$$G' = P_4 B_{n-1} + w_2 P_3 Y_{n-1} \qquad (1)$$

and

$$G'' = P_3 Y_{n-1} + w_2 P_2 R_{n-1}. \qquad (2)$$

It can be easily confirmed that B_n contains 4n+2 nodes. Also, the proper cycles that contain uw will be those consisting of all the edges (omitting the common ones) of the consecutive cells k, k + 1, k + 2,..., n-1 n, where $1 \leq k \leq n$. Each such cycle is characterized by a chain P_m containing edges not belonging to cell n and with terminal nodes u and r, where m = 4i + 2, for i = 0, 1,2,..., n-2.

This chain P_m, together with the remaining 5 edges of cell n constitute the cycle. Hence each proper cycle containing uw will contain 4i + 6 nodes. The graph obtained from B by removing such a cycle, will be a graph of type R_r, where r = n-i-1. Hence we have the following result for the graph G*.

$$G^* = \sum_{i=0}^{n-1} w_{4i+6} R_{n-i-1} . \qquad (3)$$

Equations (1), (2) and (3) together with Theorem 1, yield the following lemma.

Lemma 6

$$B_n = P_4 B_{n-1} + 2w_2 P_3 Y_{n-1} + w_2^2 P_2 R_{n-1} + \sum_{i=0}^{n-1} w_{4i+6} R_{n-i-1} \ (n>1) .$$

Apply the reduction process to the graph R_n, using the edge ab. The graph G′ will be X_n. G′′ will be the graph obtained from B_{n-1} by attaching P_2 and P_4 to the nodes of a terminal edge. In this case, we have C(G*) = 0. Applying the reduction process to the graph G′′ using the edge adjacent to nodes of valencies 1 and 2, we get

$$G'' = w_1 Y_{n-1} + w_2 R_{n-1} .$$

Hence

$$R_n = w_1 X_n + w_1 w_2 Y_{n-1} + w_2^2 R_{n-1} . \qquad (4)$$

Applying the reduction process to the graph X, using ab, and to Y_n, using bc, yield

$$X_n = w_1 B_n + w_2 Y_{n-1} \qquad (5)$$

and

$$Y_n = w_1 R_n + w_2 X_n . \qquad (6)$$

Equation (5) by w_1 added to Equation (4), yields

$$2w_1 w_2 Y_{n-1} = -w_1^2 B_{n-1} + R_n - w_2^2 R_{n-1} . \qquad (7)$$

Hence, by substituting in Lemma 6 for P_3, P_4 and Y_{n-1}, we get

Theorem 3

$$B_n = w_2(w_1^2 + w_2)\, B_{n-1} + (w_1^2 + 2w_2)\, R_n - w_2^3\, R_{n-1} + \sum_{i=0}^{n-1} w_{4i+6}\, R_{n-i-1} \quad (n>0),$$

with $B_0 = w_1^2 + w_2$ and $R_0 = 1$ and R_s (s>0) is given below in Table 1.

Let us apply the reduction process to the graph R_n by deleting edge ac (see Figure 2). In this case, G′ will be the graph R_{n-2} with two equal chains P_4 attached to a terminal edge. This graph will be denoted by $\underline{H_{n-2,4}}$. The graph G′′ will be R_{n-1}, together with two isolated nodes.

Therefore

$$G'' = P_1^2\, R_{n-1} = w_1^2\, R_{n-1}. \tag{8}$$

The restricted graph will be similar to G* of Equation (3), except for two isolated nodes. Hence we will get (see Equation (3)).

$$G^* = w_1^2 \sum_{i=0}^{n-2} w_{4i+6}\, R_{n-i-2}\ . \tag{9}$$

Let us apply the reduction process to $H_{n-2,4}$, by deleting the edge to which the two chains are attached. This yields

$$H_{n-2,4} = H_{n-3,6} + w_2\, P_3^2\, R_{n-3} + P_3^2 \sum_{i=0}^{n-3} w_{4i+6}\, R_{n-i-3}. \tag{10}$$

(c.f. Equations (8) and (9)).

By using Equation (10) recursively, until we obtain the graph $H_{0,2n}$ (which is P_{4n}), we obtain the following equation:

$$G' = H_{n-2,4} = P_{4n} + w_2 \sum_{j=1}^{n-2} P^2_{2n-2j-1}\, R_j + \sum_{j=1}^{n-2}[P^2_{2n-2j-1} \sum_{i=0}^{j-1} w_{4i+6}\, R_{j-i-1}] \quad (n>1). \tag{11}$$

Notice that when j=n-1, the terms inside the summations over j, become the expressions given in Equations (8) and (9) respectively. Hence by using Theorem 1 with G′′, G* and G as given in Equations (8), (9) and (11) respectively, we obtain the following result.

Theorem 4

$$R_n = P_{4n} + \sum_{j=1}^{n-1} \{P^2_{2n-2j-1}\ [w_2 R_j + \sum_{i=1}^{j-1} w_{4i+6}\ R_{j-i-1}]\}(n>1),$$

where

$$R_1 = w_1{}^4 + 3w_1{}^2 w_2 + w_2{}^2 \text{ and } R_0 = 1.$$

Theorems 3 and 4 can be used to obtain explicit formulae for the circuit polynomials of benzene chains. Since the coefficients of $C(B_n)$ are the numbers of the different cycle decompositions of B_n, we have obtained the necessary results for deducing the numbers of the different cycle decompositions of B_n, for all values of n.

We have used Theorems 3 and 4 in order to construct the following tables (The computations were extremely tedious!).

Table 1

Circuit Polynomials of the Graphs R_n

n	$C(R_n;\underline{w})$
1	$w_1^4+3w_1^2w_2+w_2^2$
2	$w_1^8+8w_1^6w_2+18w_1^4w_2^2+11w_1^2w_2^3+w_2^4+w_1^2w_6$
3	$w_1^{12}+13w_1^{10}w_2+60w_1^8w_2^2+119w_1^6w_2^3+97w_1^4w_2^4+26w_1^2w_2^5+w_2^6+2w_1^6w_6+8w_1^4w_2w_6+5w_1^2w_2^2w_6+w_1^2w_{10}$
4	$w_1^{16}+18w_1^{14}w_2+127w_1^{12}w_2^2+447w_1^{10}w_2^3+827w_1^8w_2^4+779w_1^6w_2^5+335w_1^4w_2^6+50w_1^2w_2^7+w_2^8+3w_1^{10}w_6+$ $26w_1^8w_2w_6+69w_1^6w_2^2w_6+60w_1^4w_2^3w_6+14w_1^2w_2^4w_6+w_1^4w_6^2+2w_1^6w_{10}+8w_1^4w_2w_{10}+5w_1^2w_2^2w10+w_1^2w_{14}$

Table 2

Circuit Polynomials of Benzene Chains

n	$C(B_n;\underline{w})$
1	$w_1^6+6w_1^4w_2^2+9w_1^2w_2^2+2w_2^3+w_6$
2	$w_1^{10}+11w_1^8w_2+41w_1^6w_2^2+61w_1^4w_2^3+31w_1^2w_2^4+2w_1^4w_6+2w_2^2w_6+6w_1^2w_2w_6+3w_2^5+w_{10}$
3	$w_1^{14}+16w_1^{12}w_2+98w_1^{10}w_2^2+290w_1^8w_2^3+429w_1^6w_2^4+294w_1^4w_2^5+76w_1^2w_2^6+$

$4w_2^7+3w_1^8w_6+22w_1^6w_2w_6+47w_1^4w_2^2w_6+28w_1^2w_2^3w_6+3w_2^4w_6+2w_1^4w_{10}+6w_1^2w_2w_{10}+2w_2^2w_{10}+w_1^2w_6^2+w_{14}$

4 $w_1^{18}+21w_1^{16}w_2+180w_1^{14}w_2^2+814w_1^{12}w_2^3+2096w_1^{10}w_2^4+3092w_1^8w_2^5+2497w_1^6w_2^6+993w_1^4w_2^7+155w_1^2w_2^8+$
$5w_2^9+4w_1^{12}w_6+48w_1^{10}w_2w_6+206w_1^8w_2^2w_6+384w_1^6w_2^3w_6+298w_1^4w_2^4w_6+80w_1^2w_2^5w_6+4w_2^6w_6+3w_1^8w_{10}+$
$22w_1^6w_2w_{10}+47w_1^4w_2^2w_{10}+26w_1^2w_2^3w_{10}+w_2^4w_{10}+2w_1^2w_6w_{10}+3w_1^6w_6^2+11w_1^4w_2w_6^2+6w_1^2w_2^2w_6^2+2w_1^4w_{14}+$
$6w_1^2w_2 2_{14}+2w_2^2w_{14}+w_{18}$

Let us write $f(R_j) = (w_1^2+2w_2)R_j - w_2^3\, R_{j-1} + \sum_{i=0}^{j-1} w_{4i+6}R_{j-i-1}$. Then from Theorem 3, we have $B_n - w_2^2\,(w_1^2+w_2)\,B_{n-1} = f(R_n)$. (12)

By using this equation recursively for B_{n-1}, B_{n-2}, etc, and applying the method of differences, we obtain the following theorem, giving $C(B_n)$ explicity in terms of the polynomials $C(R_j)$.

<u>Theorem 5</u>

$$C(B_n) = w_2^n(w_1^2+w_2)^{n+1} + \sum_{j=1}^{n} [w_2(w_1^2+w_2)]^{n-j}\ f(C(R_j))\ \ (n>0).$$

4. CHARACTERISTIC POLYNOMIALS OF BENZENE CHAINS

Using Lemma 2 together with Theorems 3,4 and 5, we obtain the following parallel results for characteristic polynomials.

<u>Corollary 3.1</u>

$$\Phi(B_n) = (1-x^2)\ \ \Phi(B_{n-1}) + (x^2-2)\Phi(R_n) + \Phi(R_{n-1}) - 2\sum_{i=0}^{n-1}\Phi(R_{n-i-1})\ \ (n>0),$$

where $\Phi(B_0) = x^2-1$ and $\Phi(R_n)$ as given below in Corollary 4.1.

<u>Corollary 4.1</u>

$$\Phi(R_n) = \Phi(P_{4n}) - \sum_{j=1}^{n-1}\{\Phi(P^2_{2n-2j-1})\ [\Phi(R_j) + 2\sum_{i=1}^{j-1}\Phi(R_{j-i-1})]\}(n>1),$$

where $\Phi(R_1) = x^4-3x^2+1$ and $\Phi(R_0) = 1$.

Corollary 5.1

$$\Phi(B_n) = -(1-x^2)^{n+1} + \sum_{j=1}^{n} (1-x^2)^{n-j} f(\Phi(R_j)) \quad (n>0),$$

where $f(\Phi(R_j)) = (x^2-2)\,\Phi(R_j) + \Phi(R_{j-1}) - 2\sum_{i=0}^{j-1}\Phi(R_{j-i-1})$.

The following tables are analogous to Tables 1 and 2 above. They give characteristic polynomials of the graphs R_n and B_n.

Table 3

Characteristic Polynomials of the Graphs R_n

n	$\Phi(R_n;x)$
1	x^4-3x^2+1
2	$x^8-8x^6+18x^4-13x^2+1$
3	$x^{12}-13x^{10}+60x^8-123x^6+113x^4-38x^2+1$
4	$x^{16}-18x^{14}+127x^{12}-453x^{10}+879x^8-921x^6+491x^4-90x^2+1$

Table 4

Characteristic Polynomials of Benzene Chains

n	$\Phi(B_n;x)$
1	$x^6-6x^4+9x^2-4$
2	$x^{10}-11x^8+41x^6-65x^4+43x^2-9$
3	$x^{14}-16x^{12}+98x^{10}-296x^8+473x^6-392x^4+148x^2-14$
4	$x^{18}-21x^{16}+180x^{14}-822x^{12}+2192x^{10}-3510x^8+3321x^6-1731x^4+411x^2-23$

We can obtain yet another recurrence for $\Phi(B_n)$, using Corollary 3.1. We have from the corollary,

$$\Phi(B_n)=(2-x^2)\,\Phi(B_{n-1})+(x^2-2)\,\Phi(R_n)+\Phi(R_{n-1})-2\Big[\sum_{i-1}^{n-1}\Phi(R_{n-i-1})\Big]-\Phi(B_{n-1})$$

$$=(2-x^2)\Phi(B_{n-1})+(x^2-2)\Phi(R_n)+\Phi(R_{n-1})-2\sum_{i=0}^{n-1}\Phi(R_{n-i-1})$$

$$-[(1-x^2)\phi(B_{n-2})+(x^2-2)+\phi(R_{n-1})+\phi(R_{n-2})-2\sum_{i=0}^{n-2}\phi(R_{n-i-2})] .$$

On simplification, this yields the following result.

Corollary 3.2.

$$\Phi(B_n) = (2-x^2)\Phi(B_{n-1}) +(x^2-1)\Phi(B_{n-2}) + (x^2-2)\Phi(R_n) + (1-x^2)\Phi(R_{n-1})$$
$$-\Phi(R_{n-2}) \quad (n>1).$$

In practice, this corollary is much better to use for finding values of $\Phi(B_n)$, since it does not involve a summation. We note that Hosoya and Ohkami [12] have given an explicit recurrence of order 4, for $\Phi(B_n)$. Their recurrence was obtained by using a matrix technique similar to that previously used in [5]. This technique works quite well for n-gon chains, when $n\leq 6$. However, for larger values of n, the method is difficult to use, because of the complicated coefficients which appear in the recurrences, and consequently appear in the matrix of coefficients.

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