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Fibonacci relations. On the computation of some counting polynomials of very large graphs

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A definition of a set of Fibonacci graphs is introduced which allows construction of several counting polynomials of very large graphs quite easily using a pencil-and-a-paper approach. These polynomials include matching, sextet, independence, Aihara and Hosoya polynomials. Certain combinatorial properties of Kekulé counts of benzenoid hydrocarbons are given. A relation to a new topological function that counts the cardinality of graph topology [23] is given.

Key words: Nonadjacent numbers—Fibonacci graphs—graph theory

1. Introduction

Application of graph theoretical methods to the theory of aromaticity [1] led to the introduction of several related counting polynomials of chemical and mathematical importance. These polynomials have the general form given by

$$P(G; X) = \sum_{k=0}^{m} \theta(G, k) \cdot f(X, k) \tag{1}$$

where $\theta(G, k)$ represents a count of k "nonadjacent structures", m is maximum value of k and $f(X, k)$ is some function of X at a particular value of k. The $\theta(G, k)$ function might assume one of the following definitions

$$\theta(G, k) = \begin{cases} p(G, k) \\ r(B, k) \\ o(G, k) \end{cases} \tag{2}$$

Dedicated to Professor Oskar E. Polansky for his enthusiastic support, participation and promotion of chemical graph theory.

where $p(G, k)$ is a k number of ways in which K_2 subgraphs can cover G so that no two of them are joint.[1] It contributes to the terms of the acyclic polynomial [2] $r(B, k)$ is called a kth resonant sextet number of the benzenoid graph B and is equal to the number of ways in which k mutually resonant but disjoint aromatic sextets are chosen from B. These numbers are the coefficients of X^k in the sextet polynomial [4]. They also enter into the structure of the Aihara polynomial [5]. Finally $o(G, k)$ is the number of selections of k independent vertices in G [6]. They form the coefficients of the independence polynomial [6]. The importance of these polynomials [7] led people to consider methods to facilitate their computation [8]. Usually a recursion formula is complemented with a computer program [9]. Even so the number of nonadjacent structures proliferates factorially with large graphs which limits the usefulness of computers [10]. In this paper we apply a very simple pencil-and-a-paper approach for obtaining $\theta(G, k)$'s of potentially very large graphs via repeated use of Fibonacci relation [11].

2. On a suggested definition of a set of Fibonacci graphs, G^f

We define $\{G_1^f, G_2^f, \ldots, G_n^f\}$, $3 \leq n \leq \infty$ as a set of Fibonacci graphs if *either* of the following conditions hold:

1) The sets $\{G_2^f - G_1^f, G_3^f - G_1^f, \ldots, G_n^f - G_1^f\}$; $\{G_3^f - G_2^f, G_4^f - G_2^f, \ldots, G_n^f - G_2^f\}$; $\{G_4^f - G_3^f, G_5^f - G_3^f, \ldots, G_n - G_3^f\}, \ldots, \{G_{i+1}^f - G_i^f, G_{i+2}^f - G_i^f, \ldots, G_n^f - G_i^f\}$, $i = 1, 2, \ldots, n-3$ correspond to the paths $\{L_1, L_2, \ldots, L_j\}$, L_k is a path containing k vertices, where $G_r - G_s$ is a graph resulting when G_s is pruned out of G_r. To illustrate this condition we consider the trees shown in Fig. 1.

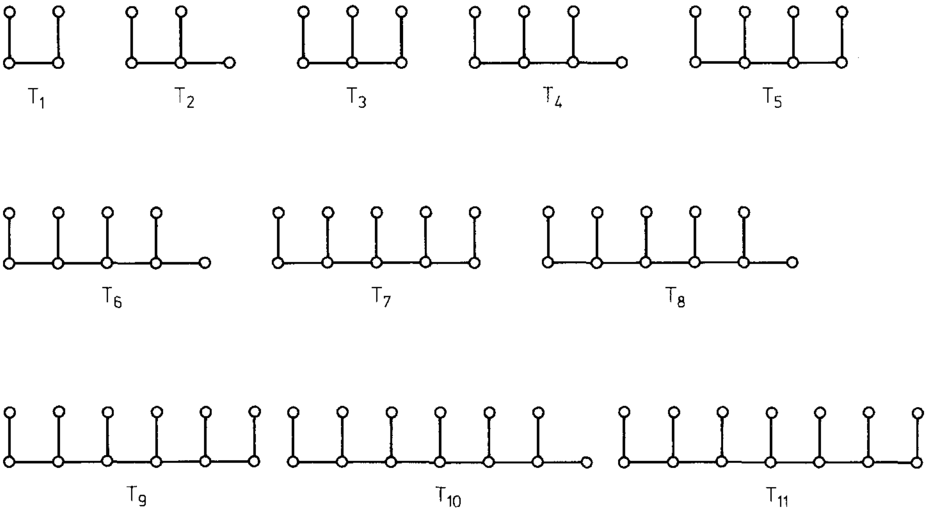

Fig. 1. Triads of Fibonacci trees

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[1] Hosoya [3] calls $p(G, k)$'s nonadjacent numbers.

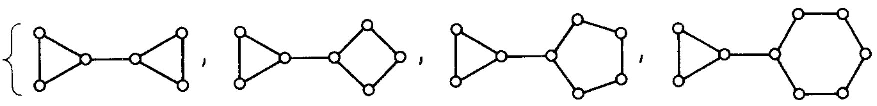
Table 1. Triads of Fibonacci trees (in braces). The numbers are $p(0), p(1), \ldots, p(m)$, 0[a]

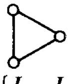
		$\sum_{k=0}^{m} p(k)$[b]
T_1	1, 3, 1, 0	5
T_2	1, 4, 2, 0	7
T_3	1, 5, 5, 1, 0	12
T_4	1, 6, 8, 2, 0	17
T_5	1, 7, 13, 7, 1, 0	29
T_6	1, 8, 18, 12, 2, 0	41
T_7	1, 9, 25, 25, 9, 1, 0	70
T_8	1, 10, 32, 38, 16, 2, 0	99
T_9	1, 11, 41, 63, 41, 11, 1, 0	169
T_{10}	1, 12, 50, 88, 66, 20, 2, 0	239
T_{11}	1, 13, 61, 129, 129, 61, 13, 1, 0	408

[a] These numbers are also $r(B, k)$'s of the benzenoid graphs shown in Fig. 3. They are also $0(G, k)$'s of the line graphs, $L(T)$'s shown in Fig. 5 (see text).
[b] These values are the Kekulé counts of the benzenoid systems of Fig. 3.

We observe that $\{T_1, T_2, T_3\}$ define a set of Fibonacci trees: $(\{T_2 - T_1, T_3 - T_1\} = \{L_1, L_2\})$. However $\{T_1, T_2, T_3, T_4\}$ is *not* a set of Fibonacci trees because while $\{T_2 - T_1, T_3 - T_1, T_4 - T_1\} = \{L_1, L_2, L_3\}$ yet $\{T_3 - T_2, T_4 - T_2\} = \{L_1, (L_1 \cdot L_1)\}$ where $(L_1 \cdot L_1)$ is a disconnected graph composed of two vertices[2]. One might factor out the following triads of Fibonacci trees (See Table 1): $\{T_1, T_2, T_3\}$; $\{T_3, T_4, T_5\}$, $\{T_5, T_6, T_7\}$; $\{T_7, T_8, T_9\}$, $\{T_9, T_{10}, T_{11}\}$.

2) Let g be a subgraph in a set of $\{G^f\}$'s. Then $\{G_1^f - g, G_2^f - g, \ldots, G_n^f - g\}$ correspond to the cycles $\{C_m C_{m+1}, \ldots, C_j\}$. E.g. in the set

2. 

…}, $g =$  , leading to the pruned set $\{C_3, C_4, C_5, \ldots\}$. One observes that the sets $\{L_0, L_1, L_2, \ldots\}$ and $\{C_3, C_4, C_5, \ldots\}$ define graphical representation of Fibonacci and Lucas sequences [12] respectively. In a set of Fibonacci graphs the following recursion exists:

$$\theta(G_m^f, k) + \theta(G_{m+1}^f, k+1) = \theta(G_{m+2}^f, k+1) \tag{3}$$

where G_m^f is a Fibonacci graph containing m vertices.

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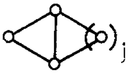
[2] Subtraction must be done by pruning the tree from left to right.

3. Results

Tables 1–5 illustrate the application of Eq. (3) to a set of G_f's. Throughout the tables $p(G, k) = p(k) = S_{2k}^{ac}$ = number of *acyclic* Sachs graphs [13] on $2k$ vertices.

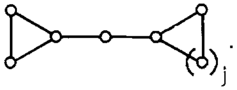
Table 2. Nonadjacent numbers, $p(k)$'s, of some annulenes



. The numbers are, from left to right, $p(0), p(1), p(2), \ldots p(m), 0$

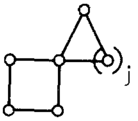
j	
1	1, 5, 2, 0
2	1, 6, 6, 0
3	1, 7, 11, 2, 0
4	1, 8, 17, 8, 0
5	1, 9, 24, 19, 2, 0
6	1, 10, 32, 36, 10, 0
7	1, 11, 41, 60, 29, 2, 0
↓	
11	1, 15, 87, 246, 350, 231, 55, 2, 0
↓	
⋮	

Table 3. Nonadjacent numbers of

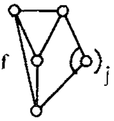


. The numbers are from left to right $p(0), p(1), p(2), \ldots, p(m), 0$

j	
1	1, 8, 17, 6, 0
2	1, 9, 24, 18, 2, 0
3	1, 10, 32, 35, 8, 0
4	1, 11, 41, 59, 26, 2, 0
5	1, 12, 51, 91, 51, 10, 0
↓	
10	1, 17, 116, 406, 761, 731, 332, 62, 2, 0
↓	
⋮	

Table 4. Nonadjacent numbers of some spiro compounds  . The numbers, from left to right, are $p(0), p(1), \ldots, p(m), 0$

j	
1	1, 7, 10, 2, 0
2	1, 8, 17, 10, 0
3	1, 9, 24, 20, 2, 0
4	1, 10, 32, 37, 12, 0
5	1, 11, 41, 61, 32, 2, 0
6	1, 12, 51, 93, 69, 14, 0
↓ ⋮	

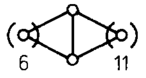
Table 5. Nonadjacent numbers of  . The numbers are from left to right $p(0), p(1), \ldots, p(m), 0$

j	
0	1, 6, 3, 0
1	1, 7, 8, 0
2	1, 8, 14, 3, 0
3	1, 9, 21, 11, 0
4	1, 10, 29, 25, 3, 0
5	1, 11, 38, 46, 14, 0
6	1, 12, 48, 75, 39, 3, 0
↓	
11	1, 17, 113, 375, 654, 574, 217, 23, 0
↓ ⋮	

4. More involved applications of Eq. 3

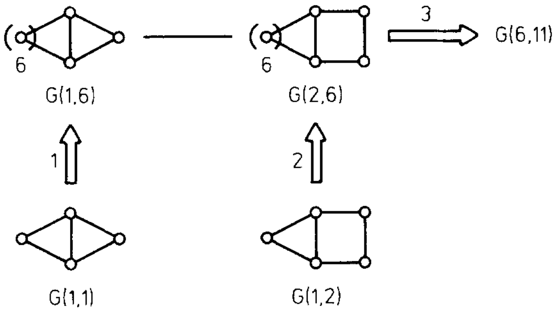
We give two examples which illustrate the more subtle points of the approach.

4.1. Calculation of nonadjacent numbers of G(6, 11)



G(6,11)

$G(6, 11)$ is a large annulene on 19 vertices. It represents an example of the explosive growth of Sachs graphs [10]. One might compute its nonadjacent numbers most easily by three sequences of what might be called *Fibonacci growth of graphs*. These sequences are graphed below:



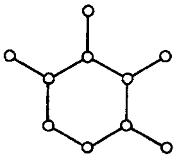
Sequences (1) and (2) involve six Fibonacci growths while sequence (3) involves nine such additions. Proceeding as in Table 2 we have the following $p(k)$'s for the leading members of sequence (3):

$G(1, 6) \Rightarrow 1, 10, 32, 36, 10, 0$

$G(2, 6) \Rightarrow 1, 11, 41, 61, 32, 3, 0.$

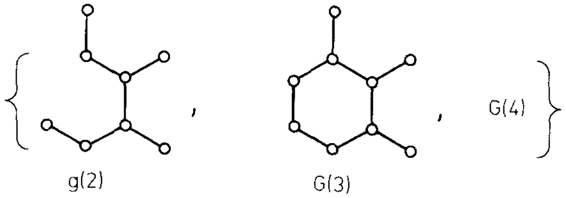
Nine applications of our recursion, Eq. 3, leads to $p(k)$'s of $G(6, 11)$, these are: 1, 20, 167, 757, 2026, 3258, 3061, 1550, 356, 25. The whole job takes about 15 minutes with a desk calculator. (The $p(k)$'s of the required leading members, $G(1, 1)$, $G(1, 2)$, $G(2, 2)$ are simply calculated either by inspection or using Heilbronner's well-known recursion [14]), thus $G(6, 11)$ has been regressed down to quite very simple graphs.

4.2. Nonadjacent numbers of G(4):



G(4)

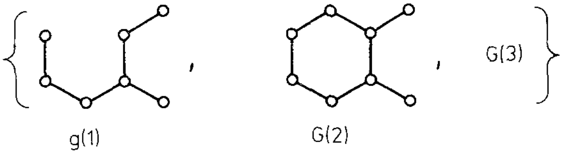
The problem lies in identifying Fibonacci graphs which precede $G(4)$. These are



The required $p(k)$'s might therefore be computed:

$g(2)$	1, 7, 13, 7, 1, 0
$G(3)$	1, 9, 24, 20, 4, 0
$G(4)$	1, 10, 31, 33, 11, 1

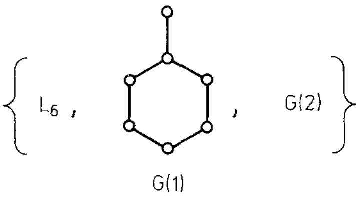
We might have obtained the $p(k)$'s of $G(3)$ by identifying its Fibonacci set:



Thus

$g(1)$	1, 6, 9, 3, 0
$G(2)$	1, 8, 18, 11, 1, 0
$G(3)$	1, 9, 24, 20, 4, 0

Again the $p(k)$'s of $G(2)$ are obtainable by identifying it in the set:



where the $p(k)$'s are:

L_6	1, 5, 6, 1, 0
$G(1)$	1, 7, 13, 5, 0
$G(2)$	1, 8, 18, 11, 1

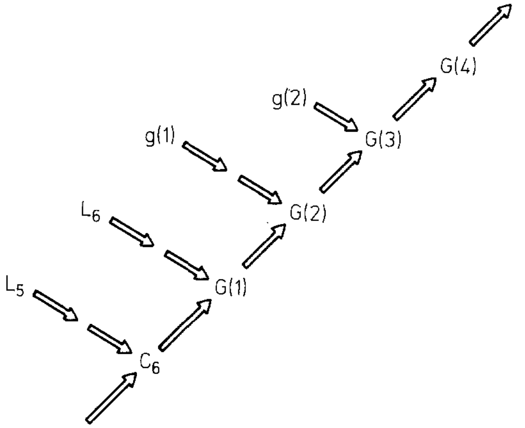


Fig. 2. Graphical synthesis of nonadjacent numbers of $G(4)$ from L_5

Finally $G(1)$ is a member of $\{L_5, C_6, G(1)\}$, whence

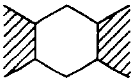
L_5	1, 4, 3, 0
C_6	1, 6, 9, 2, 0
$G(1)$	1, 7, 13, 5, 0

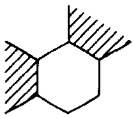
The method is illustrated in Fig. 2.

So, all graphs, in principle, might be regressed down to very small ones and this is the concept of the approach. Such a concept finds analogy with Balasubramanian's scheme [15] of reducing secular determinants to those of his quotient trees.

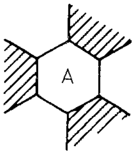
5. On Resonant Sextet numbers [4], $r(B, k)$'s of large Cata-Condensed Benzenoid hydrocarbons

First we cite some terminology: A molecular network which is entirely composed of hexagons is called *benzenoid.* If all benzene rings in one of the Kekulé structures had an aromatic sextet the hydrocarbon is called *all-benzenoid.* If *no* three hexagons have a common atom, the system is called Cata-condensed. If every hexagon of a cata-condensed system has at most two neighboring hexagons, it is said to be *nonbranched.* If there is at least one hexagon in a cata-condensed hydrocarbon that is surrounded by three other hexagons, it is said to be branched. The nonterminal hexagons in a nonbranched cata-condensed system can be anellated in just two ways [16], viz.

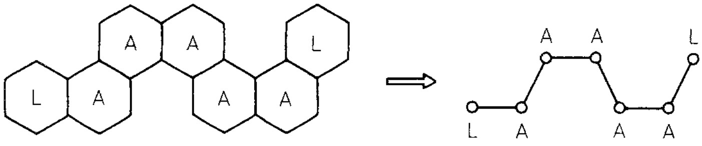

L-mode


A-mode

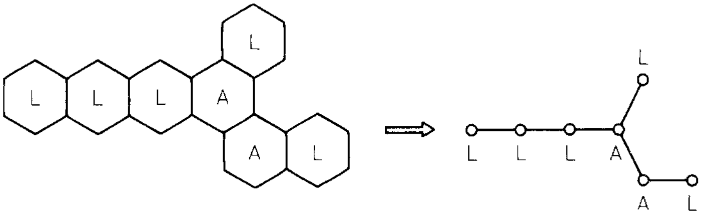
The Symbols L and A refer to linear and angular respectively. We shall adopt the additional convention that a branched hexagon will be assigned the symbol A, viz.,



A dualist [17], $D(B)$, of a benzenoid hydrocarbon results when its hexagons are replaced by vertices and then connecting adjacent vertices corresponding to rings which had a common edge in the benzenoid graph, B. Thus a benzenoid hydrocarbon containing R rings (as well as its corresponding $D(B)$ containing R vertices) might be associated with an ordered R-tuple of L, A symbols (depending on modes of anellation of rings). As usual we adopt the convention that terminal rings be given the symbol L, we illustrate the above concepts with the following examples



a nonbranched all-benezoid cata-condensed system and its dualist



a branched non-all-benzenoid cata-condensed hydrocarbon and its dualist.

6. On Gutman trees [16]

Gutman [16], in his search for methods to facilitate computation of sextet polynomials of complex nonbranched cata-condensed hydrocarbons, associated a tree with every L, A sequence given to the rings of the hydrocarbon. He then proved the identity

$$r(B, k) = p(T, k) \tag{4}$$

where $T = T(B)$, i.e. the tree corresponding to B. *Not all trees, however, are transformable into benzenoid graphs* [18]. We shall call a tree, $T = T(B)$, a *Gutman tree,* which is simply formed by the addition of an arbitrary number of vertices to an arbitrary path. The details of transforming a nonbranched benzenoid graph

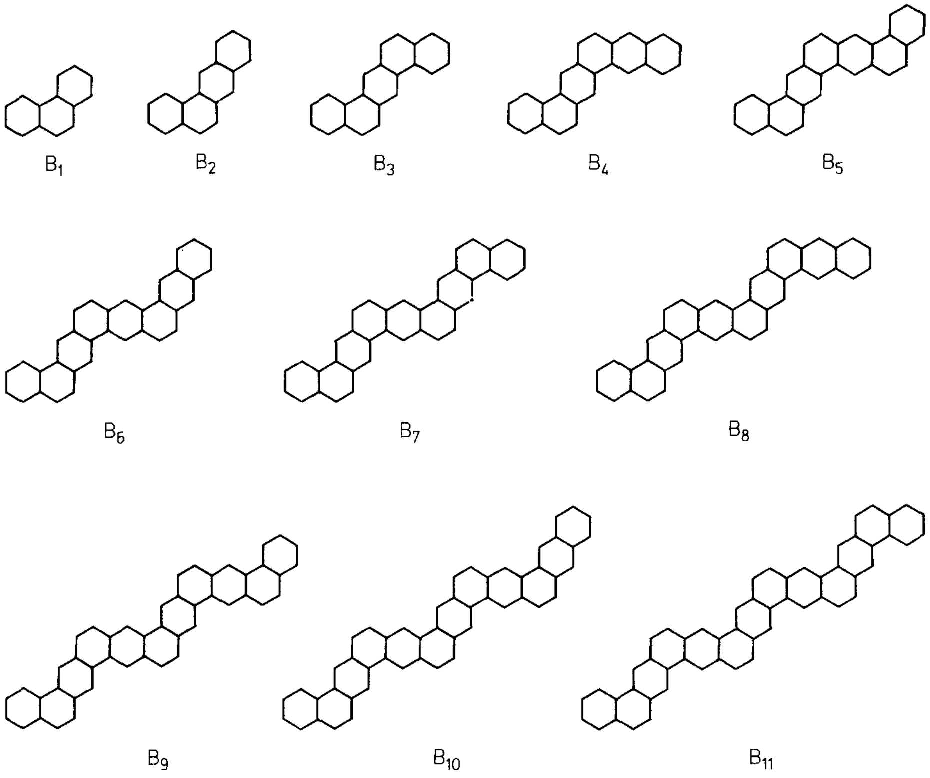


Fig. 3. Triads of Fibonacci (Benzenoid) graphs: $\{B_1, B_2, B_3\}, \{B_3, B_4, B_5\}, \ldots, \{B_9, B_{10}, B_{11}\}$

into the corresponding Gutman trees is described in Refs. [16, 19]. The trees shown in Fig. 1 are in fact one type of $T(B)$'s. They correspond to the following benzenoid graphs [16, 18, 19] (B_j corresponds to T_j of Fig. 1).

Since the $p(k)$'s of $T_1 - T_{11}$ (Fig. 1) correspond to $r(B, k)$'s of their benzenoid graphs, $B_1 - B_{11}$, we might select sets of triads of these B's whose $r(B, k)$'s satisfy recursion relation 3 and thus call them Fibonacci benzenoid graphs, B^f's. Such triads of B^f's are (B_1, B_2, B_3), (B_3, B_4, B_5), $(B_5, B_6, B_7), \ldots, (B_9, B_{10}, B_{11})$. Every subset satisfy the following relation: (a special form of Eq. 3)

$$r(B^f_R, k) + r(B^f_{R+1}, k+1) = r(B^f_{R+2}, k+1). \qquad (5)$$

Where B^f_R is a benzenoid Fibonacci graph containing R rings. *Thus the numbers in Table* 1 *are resonant sextet numbers of* $B_1 - B_{11}$ (cf. Gutman's identity, Eq. 4). One observes that B_{11} has thirteen rings and its corresponding $T(B) = T_{11}$ has fourteen vertices. This is already too large (for a pencil-and-a-paper method). However B_{11} might be regressed down to B_1, i.e. simply phenanthrene! This is shown graphically in Fig. 4.

The diagram of Fig. 4 is suggestive of an elegant way of computing the number of Kekulé structures, $K(B)$'s. Let $K_j = K(B_j)$, then, we observe that: $K_4 = K_3 + K_1$,

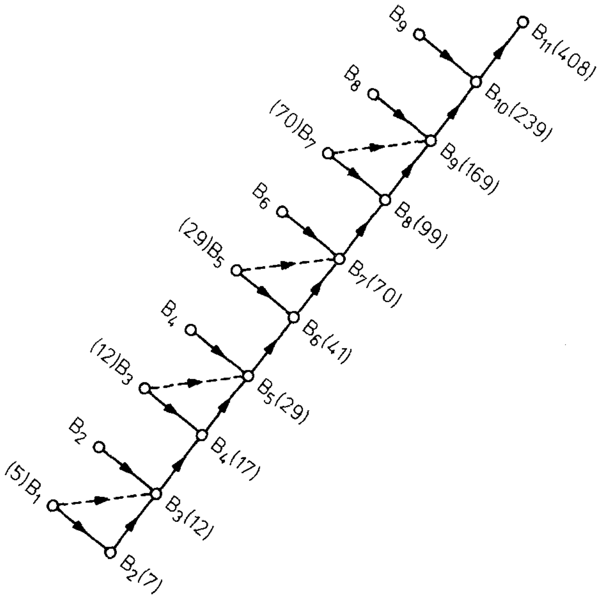


Fig. 4. Computation of resonant sextet numbers of B_{11} by regression to B_1 (phenanthrene) via repeated use of Eq. (5). Numbers in parentheses are Kekulé counts, $K(B)$'s

$K_6 = K_5 + K_3$; $K_8 = K_7 + K_5$ and $K_{10} = K_9 + K_7$. But we know that $K_3 = K_1 + K_2$; $K_5 = K_3 + K_4$; $K_7 = K_5 + K_6$; $K_9 = K_7 + K_8$ and $K_{11} = K_9 + K_{10}$. The two types of equality lead to the hierarchy of K's shown. This is equivalent to identifying the following triads of Fibonacci (benzenoid) graphs: $\{B_1, B_2, B_3\}$, $\{B_3, B_4, B_5\}$, $\{B_5, B_6, B_7\}$, $\{B_7, B_8, B_9\}$ and $\{B_9, B_{10}, B_{11}\}$. The other series being: $\{B_1, B_3, B_4\}$, $\{B_3, B_5, B_6\}$, $\{B_5, B_7, B_8\}$ and $\{B_7, B_9, B_{10}\}$. This may be realised easily *recognizing a set of benezoid graphs to be Fibonacci graphs only if their corresponding Gutman trees form a set of Fibonacci graphs.*

7. Line graphs of $T(B)$'s, $L(T(B))$'s

Fig. 5 shows $L(T(B))$'s i.e. line graphs [19, 20] of $T(B)$'s shown in Fig. 1. Gutman [19] demonstrated that

$$L(T(B)) = C(B) = C \qquad (5)$$

where C is the so called *Clar graph* [19]. The C graph corresponding to a benzenoid hydrocarbon containing R rings has R vertices: $v_1, v_2, \ldots, v_R$, such that v_i and v_j of C are adjacent (connected) if and only if the corresponding hexagons are mutually not resonant. The numbers of Table 1 correspond to $o(C, k)$'s i.e.

$$p(T_i, k) = o(C_i, k) \qquad (6)$$

Once we recognize sets of Fibonacci trees we have an easy method of computing terms of independence polynomials of Clar graphs of very large sizes. These graphs

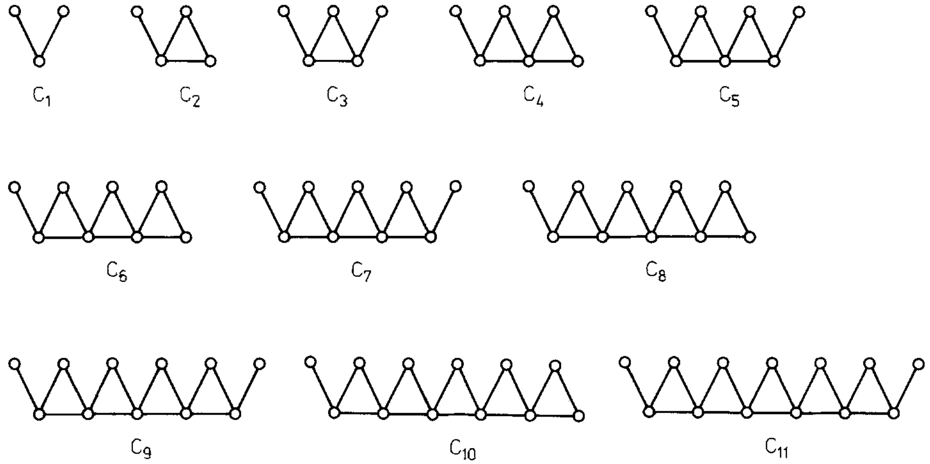


Fig. 5. Sets of Fibonacci Clar graphs. C_i corresponds to T_i (Fig. 1)and B_i (Fig. 3). The independence numbers, $o(C, k)$'s, are given in Table 1

have recently been shown [6] to be very useful for computing sextet polynomials of complex benzenoid systems.

8. All-benzenoid cata-condensed hydrocarbons

This very particular class is characterised by certain properties which make the computation of their sextet polynomials quite easy for very large systems: (1) their dualists [17], $D(B)$'s, contain *only* three types of *induced* subgraphs [20], *biz.* $\langle d_1\rangle = LA$, $\langle d_2\rangle = A^2$ and $\langle d_3\rangle = AL$. (2) The number of vertices of $\langle d\rangle$, the induced subgraph is always 2. (This is not so with non-all-benzenoids). (3) There is *only one* resonant sextet in each $\langle d\rangle$. (This property is common to other cata-condensed systems), and thus from the definition of resonant sextet numbers and sets of independent vertices we have:

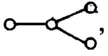
$$o(D(B), k) = r(B, k) \tag{7}$$

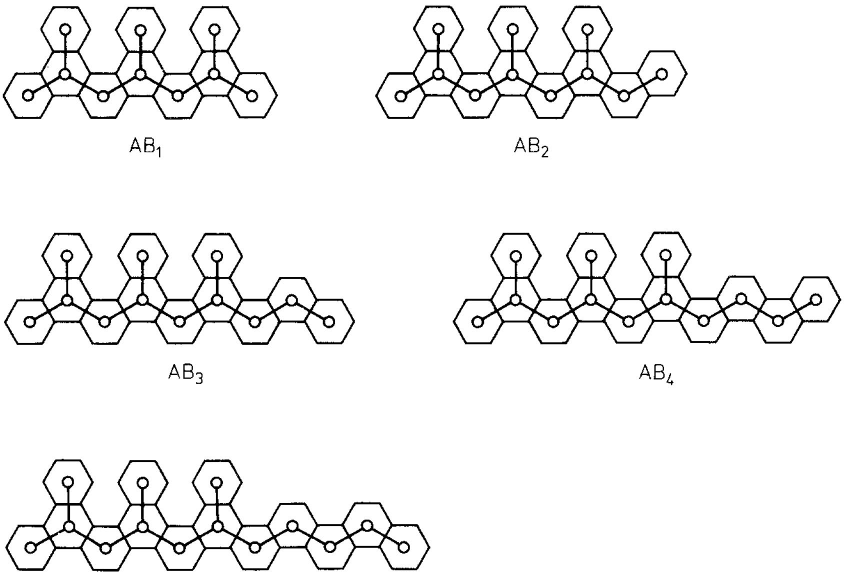
where, for all-benzoid hydrocarbons $D(B)$ has the same adjacency as $C(B)$ i.e. $C(B)$ coincides with the corresponding inner dual [21]. Thus we may write for this class of benzenoid hydrocarbons:

$$L^{-1}(D(B)) = L^{-1}(C(B)) = T(B) \tag{8}$$

where, as usual, $L^{-1}(D(B))$ is a graph, the line graph of which is $D(B)$. Whence

$$p(L^{-1})(D(B), k)) = r(B, k) = o(D(B), k). \tag{9}$$

Eq. (9) holds only for *nonbranched* all-benzenoid systems, while for branched systems $L^{-1}(D(B))$ does *not* exist, because the dualist (as well as the inner dual) of a branched cata-condensed benzenoid hydrocarbon contains , a forbidden subgraph for line graph [20].



AB$_1$ AB$_2$ AB$_3$ AB$_4$ AB$_5$

Fig. 6. A set of branched all-benzenoid, (*AB*), Fibonacci graphs and their dualists (embedded inside the hexagons). The numbers in Table 6 are $r(AB, k)$'s $= o(D, k)$'s

Table 6. Resonant sextet numbers of complex branched all-benzenoid hydrocarbons shown in Fig. 6. The entries from left to right are $r(AB, 1)$, $r(AB, 2), \ldots, r(AB, m), 0$. The numbers are also $O(D, 1), O(D, 2), \ldots$, $O(D, m)$, O where *AB* is an all-benzenoid hydrocarbon and *D* its dualist (cf. Eqs. 10, 11). Kekulé counts, *K*'s, are also given

												K
AB$_1$	1,	10,	36,	59,	49,	24,	7,	1,	0			187
AB$_2$	1,	11,	45,	87,	86,	46,	14,	2,	0			292
AB$_3$	1,	12,	55,	123,	145,	95,	38,	9,	1,	0		479
AB$_4$	1,	13,	66,	168,	232,	181,	84,	23,	3,	0		771
AB$_5$	1,	14,	78,	223,	355,	326,	179,	61,	12,	1,	0	1250[a]

[a] One observes that the construction of these resonant sextet numbers of AB_5 by method of Hosoya and Yamaguchi [4] would require drawing $1250 \times 14 = 17\,500$ hexagons!

(4) Since the Gutman trees, $T(B)$'s, of a set of nonbranched all-benzenoid hydrocarbons, $B_R, B_{R+1}, B_{R+2}, \ldots$, where B_R contains R rings, correspond to the paths $L_{R+1}, L_{R+2}, L_{R+3}, \ldots$. They define a set of Fibonacci trees, and whence:

$$r(B^f_R, k) + r(B^f_{R+1}, k+1) = r(B^f_{R+2}, k+1) \tag{10}$$

where the superscript emphasizes the Fibonacci-type recursion. Thus the terms in the independence polynomials of the corresponding dualists obey the relation:

$$O(D^f_v, k) + O(D^f_{v+1}, k+1) = O(D^f_{v+2}, k+1) \tag{11}$$

(5) For a set of branched all-benzenoids, Eqs. (10) and (11) still apply provided the set of $\{D\}$'s define a series of Fibonacci graphs. Table 6, (Fig. 6), contains an example of $\{D^f\}$'s with three branched centres. The entries of Table 6 are resonant sextet numbers of the corresponding benzenoid hydrocarbons which are also independence numbers of the corresponding dualists.

3. Conclusion

The approach presented here depends on identifying sets of Fibonacci graphs and applying Fibonacci recursion to obtain terms in their counting polynomials. Thus any graph might in principle be regressed down to its leading Fibonacci graph. The method offers an easy way of obtaining matching (characteristic) polynomials of potentially very large graphs (trees). Since certain types of trees (Gutman trees) are transformable into benzenoid hydrocarbons we, also, have a feasible method of computing sextet polynomials (and Kekulé counts) of very large hydrocarbons.

The concept of a nonadjacent structure upon which this paper is focused, and which was introduced by Hosoya [3, 4] into the chemical literature has its origins in bond eigenfunctions in relation to spin theory [22]. Such a nonadjacent function was symbolised by $\theta(G, k)$ in the present work and corresponds to a recently defined topological function [23], called $\sigma(G)$, as the cardinality of the graph topology of G i.e. is equal to the number of stable sets [23] of G.

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