FIBONACCI NUMBERS AND ALGEBRAIC STRUCTURE COUNT OF SOME NON-BENZENOID CONJUGATED POLYMERS

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1. INTRODUCTION

The algebraic structure count (ASC) of a graph G is

$$\mathrm{ASC}\{G\} \stackrel{\text{def}}{=} \sqrt{|\det A|},$$

where A is the adjacency matrix of G. This quantity has noteworthy applications in chemistry (see below), provided that the graph G represents the carbon-atom skeleton of a molecule of a class of hydrocarbons, the so-called *conjugated hydrocarbons* [9]. Therefore, we call this graph by the same name as the respective hydrocarbon.

Of particular importance for chemical applications are graphs that are connected, bipartite, and planar and which, when considered as plane graphs, have the property that every face-boundary (cell) is a circuit of length of the form $4s+2$ $(s = 1, 2, \ldots)$ [2]. We refer to these graphs as *benzenoid*, noting, however, that the actual definition of benzenoid systems is slightly more complicated [8]. Molecular graphs that are connected, bipartite, and planar, but in which some face-boundaries are circuits of length of the form $4s$ $(s = 1, 2, \ldots)$ will be referred to as *non-benzenoid*. The graphs studied in the present work belong to this latter class.

In the case of benzenoid graphs, the ASC-value coincides with the number of perfect matchings (1-factors), which is a result of crucial importance for chemical applications. Chemists call the 1-factors *Kekulé structures* [3], and these objects play significant roles in various chemical theories [8]. The enumeration of 1-factors in benzenoid graphs is not too difficult a task [3] and can be accomplished by various recursive methods. Consequently, the calculation of ASC of benzenoid graphs is easy.

In the case of non-benzenoid graphs, the relation between ASC and the number of perfect matchings is less simple and is given below (Theorem 2). Contrary to the former case, in this case the determination of the ASC-value is a nontrivial task because no efficient recursive graphical technique is known for computing ASC [5]. A systematic study of the ASC-values of non-benzenoid conjugated systems was recently initiated by one of the present authors (see [6], [7]). Among others, in [7], the linear [n]phenylene [Fig. 1(a)] and the angular [n]phenylene [Fig. 1(b)] are considered.

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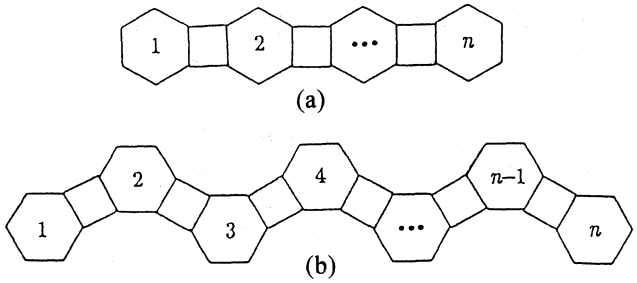

FIGURE 1

The Linear [*n*]Phenylene (a) and the Angular [*n*]Phenylene (b); Algebraic Structure Counts of Angular Phenylenes are Fibonacci Numbers

It is established that the ASC-value of the angular [*n*]phenylene is equal to the $(n+2)^{\text{th}}$ Fibonacci number ($F_0 = 0,\ F_1 = 1,\ F_2 = 1, \ldots$). It has been known for a long time [3] that the number of 1-factors (*K*-value) of the zig-zag chain $A(n)$ of n hexagons (circuits of length 6) (Fig. 2) is equal to the same number, i.e.,

$$K\{A(n)\} = F_{n+2}. \tag{1}$$

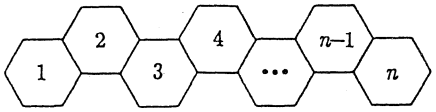

FIGURE 2

The Zig-Zag Hexagonal Chain $A(n)$; Number of 1-Factors of $A(n)$ Is a Fibonacci Number

In this paper we show that the ASC-value of a class of non-benzenoid hydrocarbons can be expressed by means of Fibonacci numbers. This structure $B_n \equiv B_n(A(m_1), A(m_2), \ldots, A(m_n))$ (which will be described in detail later) consists of n zig-zag chains concatenated by $(n-1)$ squares (circuits of length 4). The manner of concatenation of two zig-zag chains by a square depends on *the types* (I-IV) of these zig-zag chains (which will also be defined later). The main result is the following statement.

Theorem 1: If the graph B_n consists of n zig-zag chains of the same length m $(m > 2)$ concatenated in the same manner, i.e., all zig-zag chains are of the same type, then

$$\mathrm{ASC}\{B_n\} = \frac{1}{2^{n+1}}\left[\left(1+\frac{F_{m+2}+F}{D}\right)(F_{m+2}-F+D)^n + \left(1-\frac{F_{m+2}+F}{D}\right)(F_{m+2}-F-D)^n\right],$$

where

$$D = \begin{cases} \sqrt{(F_{m+2}-F_{m-2})^2 + 4\cdot(-1)^{m+1}}, & \text{if } A(m) \text{ is of type I,} \\ \sqrt{(F_{m+2}-F_{m-1})^2 + 4\cdot(-1)^{m}}, & \text{if } A(m) \text{ is of type II or III,} \\ \sqrt{F_{m+1}^2 + 4\cdot(-1)^{m+1}}, & \text{if } A(m) \text{ is of type IV,} \end{cases}$$

and

$$F = \begin{cases} F_{m-2}, & \text{if } A(m) \text{ is of type I,} \\ F_{m-1}, & \text{if } A(m) \text{ is of type II or III,} \\ F_m, & \text{if } A(m) \text{ is of type IV.} \end{cases}$$

Before proving the validity of Theorem 1, we wish to mention a few more chemical aspects of the ASC-concept [4].

First of all, ASC is a well-defined quantity only for molecular graphs that are bipartite. There are two basic applications of ASC. First, if ASC = 0, then the respective conjugated hydrocarbon is predicted to have unpaired electrons. In practice, this means that this hydrocarbon is extremely reactive and usually does not exist. Second, thermodynamic stability of conjugated hydrocarbons is related to, and is a monotone increasing function of the ASC-value of the underlying molecular graph. In practice, this means that among two isomeric conjugated hydrocarbons, the one having greater ASC will be more stable. (Recall that the molecular graphs of isomeric hydrocarbons have an equal number of vertices and an equal number of edges.)

In the case of benzenoid hydrocarbons, the above remains true if ASC is interchanged by K, the number of 1-factors [8]. In particular, not a single benzenoid hydrocarbon with $K = 0$ is known, whereas many hundreds of such hydrocarbons with $K > 0$ exist.

In the case of benzenoid hydrocarbons, the following example (kindly suggested by the anonymous referee) illustrates another aspect of the role of 1-factors. Consider two isomers, A and B, consisting of n fused benzene rings (i.e., hexagons). Compound A consists of a linear arrangement of hexagons, and possesses $n+1$ Kekulé structures (1-factors). Compound B consists of a zig-zag arrangement of n hexagons (see Fig. 2); it possesses F_{n+2} Kekulé structures. The electron distribution in compounds A and B can be (as a reasonable approximation) obtained by averaging of the Kekulé structures [8]. By means of this approach, one finds that compound A has very nearly double bonds at its ends (i.e., bonds the order of which is about 2), which implies a relatively high reactivity in this region of the molecule. In the case of compound B, the same averaging results in bond orders 1.618 (the golden ratio) at the terminal bonds, implying a significantly greater chemical stability of B relative to A.

Readers interested in further details of the chemical applications of 1-factors (including the theory of ASC) should consult the references quoted.

2. COUNTING THE ASC-VALUE OF A BIPARTITE GRAPH

Consider a bipartite graph G with $n+n$ vertices, i.e., a graph all of whose circuits are of even length. Define a binary relation ρ in the set of all 1-factors of G in the following way.

Definition 1: The 1-factors k_1 and k_2 are in relation ρ if and only if the union of the sets of edges of k_1 and k_2 contains an even number of circuits whose lengths are all multiples of 4.

It can be proved that this binary relation is an equivalence relation and subdivides the set of 1-factors into two equivalence classes [2]. In [2] this relation is called "being of the same parity" and the numbers of these classes are denoted by K_+ and K_-. The following theorem by Dewar and Longuet-Higgins [2] connects the ASC-value of G and the numbers K_+ and K_-.

Theorem 2: $\det A = (-1)^n (K_+ - K_-)^2$.

This theorem implies $\mathrm{ASC}\{G\} = \sqrt{|\det A|} = |K_+ - K_-|$.

In the case of benzenoid hydrocarbons all 1-factors are in the same class, i.e., one of the numbers K_+ or K_- is equal to zero. This follows directly from Definition 1. Hence, $\mathrm{ASC}\{G\} = K\{G\}$. It does not hold in the case of non-benzenoid hydrocarbons. In this case, the following theorem can be useful for evaluating the ASC-value.

Theorem 3: Two 1-factors k_1 and k_2 are in distinct classes (of opposite parity) if one is obtained from the other by cyclically rearranging an even number of edges. In other words, two 1-factors k_1 and k_2 are in distinct classes if the union of the sets of edges of k_1 and k_2 contains just a single circuit, and the length of this circuit is a multiple of 4.

Proof: Theorem 3 follows directly from Definition 1.

3. THE STRUCTURE OF THE CONSIDERED GRAPH

The graph $B_n \equiv B_n(X_1, X_2, \ldots, X_n)$ considered in this paper is obtained from the linear $[n]$phenylene [Fig. 1(b)] by replacing its i^{th} hexagon with a zig-zag chain, labeled by X_i $(X_i = A(m_i))$ for $i = 1, \ldots, n$ [Fig. 3(a)]. The places of concatenation are the edges $f_i \equiv p_i q_i$ $(i = 2, \ldots, n)$ and $g_i \equiv r_i s_i$ $(i = 1, 2, \ldots, n-1)$ which belong to the terminal hexagons of the zig-zag chain. In the graph B_n, the valencies of the vertices p_i, q_i, r_{i-1}, and s_{i-1} $(i = 2, 3, \ldots, n)$ are equal to 3. Recall that the notation $B_n(A(m_1), A(m_2), \ldots, A(m_n))$ does not uniquely determine a graph, because for a unique characterization the places of concatenations also need to be specified (as discussed in detail below).

Figure 3(b) shows one of the possible structures of the graph $B_4(A(3), A(4), A(4), A(2))$.

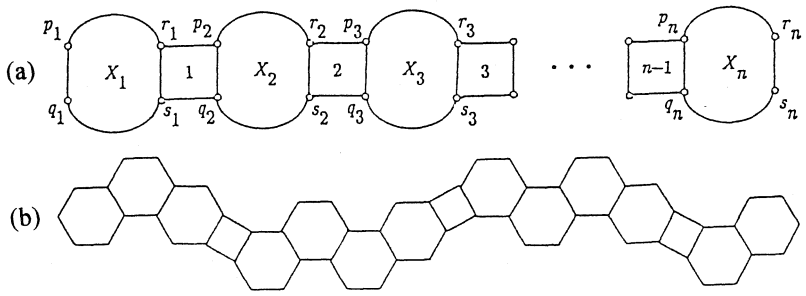

FIGURE 3

The Graph $B_n \equiv B_n(X_1, X_2, \ldots, X_n)$ (a) and Its Special Case $B_4(A(3), A(4), A(4), A(2))$ (b); Note that the Symbol $B_4(A(3), A(4), A(4), A(2))$ Does Not Specify a Unique Graph

The present authors considered in [1] the generalization of the structure of the type B_n [Fig. 3(a)], where X_i are arbitrary bipartite graphs all of whose 1-factors are of equal parity, i.e., $\mathrm{ASC}\{X_i\} = K\{X_i\}$

Consider now a zig-zag segment $A(m_i)$ of B_n. Let $m_i = 1$. Then (see Fig. 4) there are two possible choices of the edges f_i and g_i depending on whether these edges are parallel or not (note that we can always represent squares and hexagons as regular k-gons).

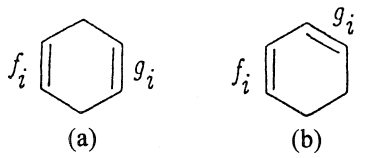

FIGURE 4

Two Ways of Choosing the Edges f_i and g_i in a Hexagon

If $m_i \geq 2$, then there are four *types* of the zig-zag chains $A(m_i)$, depending on the choices of the edges f_i and g_i, according to whether or not these edges are parallel to the edge in common of the hexagon containing the considered edge and its adjacent hexagon (see Fig. 5).

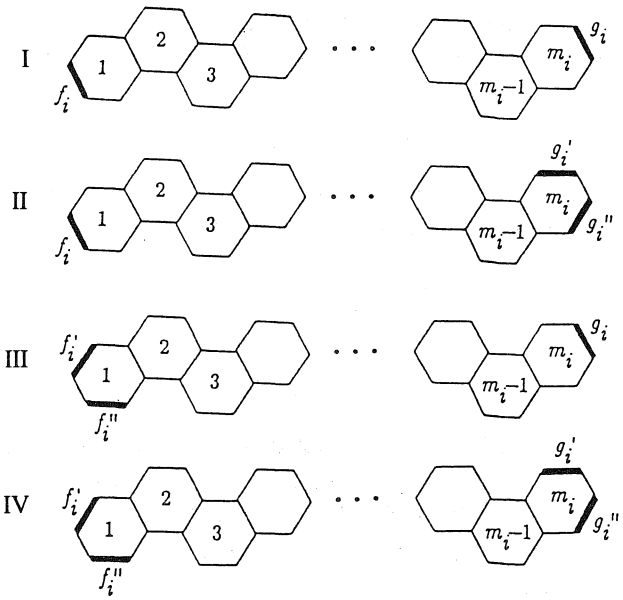

FIGURE 5

Four Ways of Choosing the Edges f_i and g_i in a Zig-Zag Chain $A(m_i)$

Note that in the type II and type III we have two possibilities for the edge pair f_i, g_i and in the type IV we have four such possibilities.

4. A METHOD FOR CALCULATING THE ASC-VALUE OF THE GRAPH B_n

Observe that edges belonging to a 1-factor of B_n (marked by double lines in Fig. 6) can be arranged in and around a four-membered circuit in exactly five different ways. This is the consequence of the fact that the fragments of B_n lying on the left- and right-hand side of the four-membered circuit (not shown in Fig. 6) both possess an even number of vertices. If the number of vertices in these fragments would be odd (which, according to the way in which B_n is constructed, is impossible), then every 1-factor of B_n would contain one horizontal edge of the four-membered circuit, and would not contain the other.

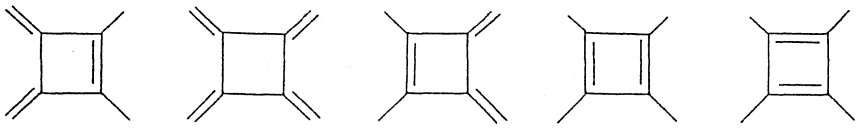

FIGURE 6

Arrangements of Edges in 1-Factors of B_n

The modes 4 and 5 are interconverted by rearranging two (an even number) edges of the 1-factor. According to Theorem 4, modes 4 and 5 are of opposite parity. Consequently, they need not be taken into account when the algebraic structure count is evaluated. The 1-factors of B_n that do not contain arrangements of mode 4 or 5 are called *good*, and their number is denoted by $\kappa\{B_n\}$. Note that the horizontal edges of squares are never in a good 1-factor. Hence, the edges of good 1-factors can be rearranged only within each fragment X_i. This implies that all good 1-factors of B_n are of equal parity, i.e.,

$$\mathrm{ASC}\{B_n\} = \kappa\{B_n\}. \tag{2}$$

We now enumerate the good 1-factors of B_n using the so-called *transfer matrix method* [2]. For that purpose, we define auxiliary subgraphs $X_{i,j}$ in the following way:

$$\left.\begin{aligned} X_{i,1} &= X_i - (f_i) - (g_i), \\ X_{i,2} &= X_i - (f_i) - g_i, \\ X_{i,3} &= X_i - f_i - (g_i), \\ X_{i,4} &= X_i - f_i - g_i. \end{aligned}\right\} \tag{3}$$

(The subgraph $G-e$ is obtained from G by deleting the edge e and the subgraph $G-(e)$ is obtained from G by deleting both the edge e and its terminal vertices.) To simplify the notation, denote $K\{X_{i,j}\}$ by $K_{i,j}$. Observe that $K_{i,1}$-$K_{i,4}$ are equal to the number of 1-factors of X_i in which one of the following four conditions is fulfilled. In particular:

- $K_{1,i}$ counts the 1-factors containing both edges f_i and g_i (we say that this class of the 1-factors of X_i is *assigned to the graph* $X_{i,1}$);
- $K_{i,2}$ counts the 1-factors containing the edge f_i and not containing the edge g_i (this class is *assigned to the graph* $X_{i,2}$);
- $K_{i,3}$ counts the 1-factors that do not contain f_i and do contain g_i (this class is *assigned to the graph* $X_{i,3}$);
- $K_{i,4}$ counts the 1-factors containing neither f_i nor g_i (*assigned to the graph* $X_{i,4}$).

Evidently, the above four cases cover all possibilities.

Now, we associate with each 1-factor of B_n a word $j_1 j_2 \ldots j_n$ of the alphabet $\{1, 2, 3, 4\}$ in the following way: *If the considered 1-factor induces in* X_i *a 1-factor that is assigned to the graph* $X_{i,j}$, *then* $j_i = j$. Note that by choosing the edges of the 1-factor in X_i and X_{i+1} (i.e., by choosing subwords $j_i j_{i+1}$) we must not generate one of modes 4 or 5 of arrangements of the 1-factor in the square between X_i and X_{i+1}, i.e., the subwords $j_i j_{i+1}$ must not belong to the set $\{11, 12, 31, 32\}$.

Let $\mathcal{T}_n$ be the set of all words in $\{1, 2, 3, 4\}^n$, in which the subwords 11, 12, 31, and 32 are forbidden. Then, according to (2), we have

$$\mathrm{ASC}\{B_n\} = \sum_{j_1 j_2 \cdots j_n \in \mathcal{T}_n} K_{1, j_1} K_{2, j_2}, \ldots, K_{n, j_n}. \tag{4}$$

It can be shown that the set $\mathcal{T}_n$ has $4 \cdot 3^{n-1}$ elements. Hence, there are $4 \cdot 3^{n-1}$ summands on the right-hand side of (4).

Let

$$M_i = \begin{bmatrix} 0 & 0 & K_{i,3} & K_{i,4} \\ K_{i,1} & K_{i,2} & K_{i,3} & K_{i,4} \\ 0 & 0 & K_{i,3} & K_{i,4} \\ K_{i,1} & K_{i,2} & K_{i,3} & K_{i,4} \end{bmatrix}.$$

Keeping (4) in mind, we see that the ASC-value of B_n is equal to the sum of all elements of the last row in the product of transfer matrices $\prod_{i=1}^{n} M_i$, i.e.,

$$\mathrm{ASC}\{B_n\} = \sum_{k=1}^{4} (M_1 \cdot M_2 \cdot \cdots \cdot M_n)_{4,k}. \tag{5}$$

In our case, the subgraphs X_i are zig-zag chains and the value $\mathrm{ASC}\{B_n\}$ is equal to the sum of the products of some Fibonacci numbers, i.e., the following statement holds.

Lemma 1: For every type of zig-zag chain $A(m_i)$, the quantities $K_{i,1}$-$K_{i,4}$ are equal to some Fibonacci numbers.

Proof: Note that all 1-factors of $A(m)$ can be divided into four classes (a)-(d) according to which edges in the terminal hexagons belong to the 1-factor (see Fig. 7). Observe that the numbers of elements in classes (a)-(d) are Fibonacci numbers F_{m-2}, F_{m-1}, F_{m-1}, and F_m, respectively. Evidently, their sum is equal to $K\{A(m_i)\}$, i.e., F_{m+2}.

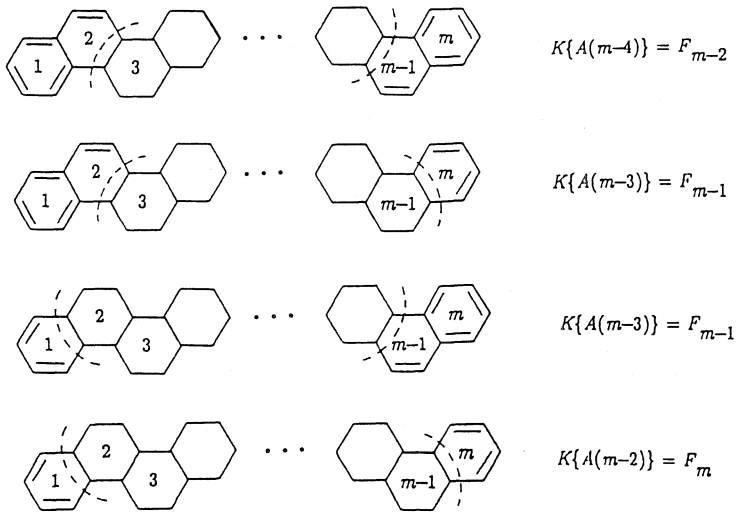

FIGURE 7

Classes of 1-Factors of $A(m)$

Now, if the zig-zag chain is of type I (Fig. 5), then the four numbers $K_{i,1}$-$K_{i,4}$ represent a cardinal number of classes (a)-(d) in Figure 7, respectively. Therefore, we can write

$$[K_{i,1},\ K_{i,2},\ K_{i,3},\ K_{i,4}] = [F_{m_i-2},\ F_{m_i-1},\ F_{m_i-1},\ F_{m_i}]\text{—for type I.} \tag{6}$$

Similarly, we obtain:

$$[K_{i,1},\ K_{i,2},\ K_{i,3},\ K_{i,4}] = [F_{m_i-1},\ F_{m_i-2},\ F_{m_i},\ F_{m_i-1}]\text{—for type II;} \tag{7}$$

$$[K_{i,1},\ K_{i,2},\ K_{i,3},\ K_{i,4}] = [F_{m_i-1},\ F_{m_i},\ F_{m_i-2},\ F_{m_i-1}]\text{—for type III;} \tag{8}$$

$$[K_{i,1},\ K_{i,2},\ K_{i,3},\ K_{i,4}] = [F_{m_i},\ F_{m_i-1},\ F_{m_i-1},\ F_{m_i-2}]\text{—for type IV.} \tag{9}$$

5. PROOF OF THEOREM 1

Let all zig-zag chains $A(m_i)$ be of the same length m $(m = m_1 = m_2 = \cdots = m_n)$ and of fixed type. Then we can write K_j instead of $K_{i,j}$ $(j = 1, \ldots, 4)$ and M instead of M_i. Then expression (5) reduces to $\mathrm{ASC}\{B_n\} = \sum_{k=1}^{4}(M^n)_{4,k}$, where

$$M = \begin{bmatrix} 0 & 0 & K_3 & K_4 \\ K_1 & K_2 & K_3 & K_4 \\ 0 & 0 & K_3 & K_4 \\ K_1 & K_2 & K_3 & K_4 \end{bmatrix}.$$

The characteristic equation of M is

$$\lambda^4 - [K_2 + K_3 + K_4]\lambda^3 + [K_2K_3 - K_1K_4]\lambda^2 = 0, \tag{10}$$

and its eigenvalues are $\lambda_1 = \lambda_2 = 0$, $\lambda_3 = [L - D]/2$, and $\lambda_4 = [L + D]/2$, where

$$L = K_2 + K_3 + K_4 \ \&\ D = \sqrt{L^2 + 4(K_1K_4 - K_2K_3)}. \tag{11}$$

Note that $D = \sqrt{(K_2 - K_3)^2 + K_4(4K_1 + 2K_2 + 2K_3 + K_4)}$ and is equal to 0 if and only if $K_2 = K_3$ and $K_4 = 0$. Further, recall the Cayley-Hamilton theorem which says that each square matrix satisfies its own characteristic equation. If we label with $m_{i,j}(n)$ the (i, j)-entry in the matrix M^n, then using the mentioned theorem we obtain that the sequence $m_{i,j}(n)$ [and, consequently, the sequence $\mathrm{ASC}\{B_n\} = \sum_{j=1}^{4} m_{4,j}(n)$] satisfies a difference equation. The coefficients of this difference equation are obtained from the characteristic polynomial of M^n, i.e., from equation (10). Thus, the desired recurrence relation for the algebraic structure count of the graph B_n is

$$\mathrm{ASC}\{B_n\} = (K_2 + K_3 + K_4)\mathrm{ASC}\{B_{n-1}\} + (K_1K_4 - K_2K_3)\mathrm{ASC}\{B_{n-2}\} \tag{12}$$

with initial conditions

$$\begin{aligned} \mathrm{ASC}\{B_1\} &= K_1 + K_2 + K_3 + K_4 \ \&\ \mathrm{ASC}\{B_2\} \\ &= (K_1 + K_3)(K_3 + k_4) + (K_2 + K_4)(K_1 + K_2 + K_3 + K_4). \end{aligned}$$

Solving the recurrence relation (12), we obtain the following general solution:

$$\mathrm{ASC}\{B_n\} = \begin{cases} (nK_1 + (n+1)K_2)K_2^{n-1} & \text{if } K_2 = K_3 \ \&\ K_4 = 0, \\ \frac{1}{2^{n+1}}\left[\left(1 + \frac{2K_1 + L}{D}\right)(L + D)^n + \left(1 - \frac{2K_1 + L}{D}\right)(L - D)^n\right] & \text{otherwise,} \end{cases} \tag{13}$$

where L and D are given by (11). We arrive at the generating function for the sequence $\mathrm{ASC}\{B_n\}$ by standard methods of the theory of difference equation

$$\mathrm{ASC}(x) = \frac{1 + K_1 x}{(K_2 K_3 - K_1 K_4)x^2 - (K_2 + K_3 + K_4)x + 1}.$$

Since $\mathrm{ASC}(x) \stackrel{\text{def}}{=} \sum_{n=0}^{\infty} \mathrm{ASC}\{B_n\} x^n$, this implies

$$\mathrm{ASC}\{B_n\} = \frac{1}{n!}\mathrm{ASC}^{(n)}(0).$$

In our case, the fragments X_i are zig-zag chains $A(m)$ with a fixed number of hexagons (m) of fixed type.

- The case $m = 1$ was considered in [7]. For the sake of completeness, we recall that
  $\mathrm{ASC}\{B_n\} = n + 1$, if $A(1)$ is of type I [Fig. 4(a)] (the linear phenylene),
  $\mathrm{ASC}\{B_n\} = F_{n+2}$, if $A(1)$ is of type II [Fig. 4(b)] (the angular phenylene).
- In the case $m = 2$, we have to use both terms in (13). So, using relations (6)-(9) in (13), we obtain

$$\mathrm{ASC}\{B_n\} = \begin{cases} \frac{1}{\sqrt{5}}\left[\left(\frac{3+\sqrt{5}}{2}\right)^{n+1} - \left(\frac{3-\sqrt{5}}{2}\right)^{n+1}\right], & \text{if } A(2) \text{ is of type I,} \\ \frac{1}{2}\left[(1+\sqrt{2})^{n+1} + (1-\sqrt{5})^{n+1}\right], & \text{if } A(2) \text{ is of type II or III,} \\ 2n+1, & \text{if } A(2) \text{ is of type IV.} \end{cases}$$

- For the case $m > 2$, all K_i ($i = 1, \ldots, 4$) numbers are positive, so we apply only the second term in (13). Bearing in mind relations (6)-(9) again and the well-known relations for the Fibonacci numbers, $F_{m-1}^2 - F_m F_{m-2} = (-1)^m$ and $F_{m-2} + 2F_{m-1} + F_m = F_{m+2}$, the required statement of Theorem 1 follows.

REFERENCES

1. O. Bodroža-Pantić, I. Gutman, & S. J. Cyvin. "Algebraic Structure Count of Some Non-Benzoid Conjugated Polymers." *Acta Chim. Hung.*, in press.
2. D. M. Cvetković, M. Doob, & H. Sachs. *Spectra of Graphs—Theory and Application*. Berlin: VEB Deutscher Verlag der Wissenschaften, 1980.
3. S. J. Cyvin & I. Gutman. *Kekulé Structures in Benzenoid Hydrocarbons*. Lecture Notes in Chemistry 46. Berlin: Springer-Verlag, 1988.
4. A. Graovac, I. Gutman, & N. Trinajstić. *Topological Approach to the Chemistry of Conjugated Molecules*. Berlin: Springer-Verlag, 1977.
5. I. Gutman. "Note on Algebraic Structure Count." *Z. Naturforsch.* **39a** (1984):794-96.
6. I. Gutman. "Algebraic Structure Count of Linear Phenylenes." *Indian J. Chem.* **32A** (1993): 281-84.
7. I. Gutman. "Easy Method for the Calculation of the Algebraic Structure Count of Phenylenes." *J. Chem. Soc. Faraday Trans.* **89** (1993):2413-16.
8. I. Gutman & S. J. Cyvin. *Introduction to the Theory of Benzenoid Hydrocarbons*. Berlin: Springer-Verlag, 1989.
9. C. F. Wilcox, Jr. "Stability of Molecules Containing Nonalternant Rings." *J. Amer. Chem. Soc.* **91** (1969):2732-36.

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