ALGEBRAIC STRUCTURE COUNT OF ANGULAR HEXAGONAL-SQUARE CHAINS

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Abstract. The algebraic structure count of a graph G can be defined by $ASC\{G\} = \sqrt{\mid detA \mid}$ where A is the adjacency matrix of G. In chemistry, thermodynamic stability of a hydrocarbon is related to the ASC-value for the graph which represents its skeleton. In the case of benzenoid graphs (connected, bipartite, plane graphs which have the property that every face-boundary (cell) is a circuit of length of the form $4s+2$ $(s = 1, 2, \ldots)$), the ASC-value coincides with $K\{G\}$ - the number of perfect matchings (Kekulé structures). However, in the case of non-benzenoid graphs (in which some cells are circuits of length of the form $4s (s = 1, 2, \ldots)$) these two numbers $ASC\{G\}$ and $K\{G\}$ can be different. Angular hexagonal-square chains (open and closed) belong to this latter class. In this paper we show that the algebraic structure count for these graphs can be expressed by means of Fibonacci and Lucas numbers.

Key words and phrases: Algebraic structure count, perfect matchings (1-factors), hexagonal chains, cyclic hexagonal-square chains

1 Introduction

The algebraic structure count of a graph G can be defined by $ASC\{G\} = \sqrt{|\, detA \,|}$ where A is the adjacency matrix of G. In chemistry, thermodynamic stability of an alternant hydrocarbon is related to the ASC-value for the bipartite graph which represents its skeleton. The basic application of ASC is in the following. Among two isomeric conjugated hydrocarbons (whose related graphs have an equal number of vertices and an equal number of edges), the one having greater ASC will be more stable. In particular, if $ASC = 0$, then the respective hydrocarbon is extremely reactive and usually does not exist [**?**, **?**].

In the case of benzenoid graphs (connected, bipartite, plane graphs which have the property that every face-boundary (cell) is a circuit of length of the form $4s + 2, \quad s = 1, 2, \ldots$), the ASC-value of the considered graph coincides with its K-value, i.e. the number of all its perfect matchings. A *perfect matching (1-factor)* of a graph G is a selection of edges of G such that each vertex of G belongs to exactly one selected edge. In chemistry, perfect matchings are called the *Kekulé structures* of the molecule whose skeleton is represented by the graph G. For example, it is known for a long time [**?**], [**?**] that the number of perfect matchings of the zig-zag chain of n hexagons (Fig.1a) is equal to the $(n + 2)$-th Fibonacci number $(F_0 = 0, F_1 = 1; F_{k+2} = F_{k+1} + F_k, \;\; k \geq 0)$ and the number of perfect matchings of the linear chain of n hexagons (Fig.1b) is equal to $n + 1$.

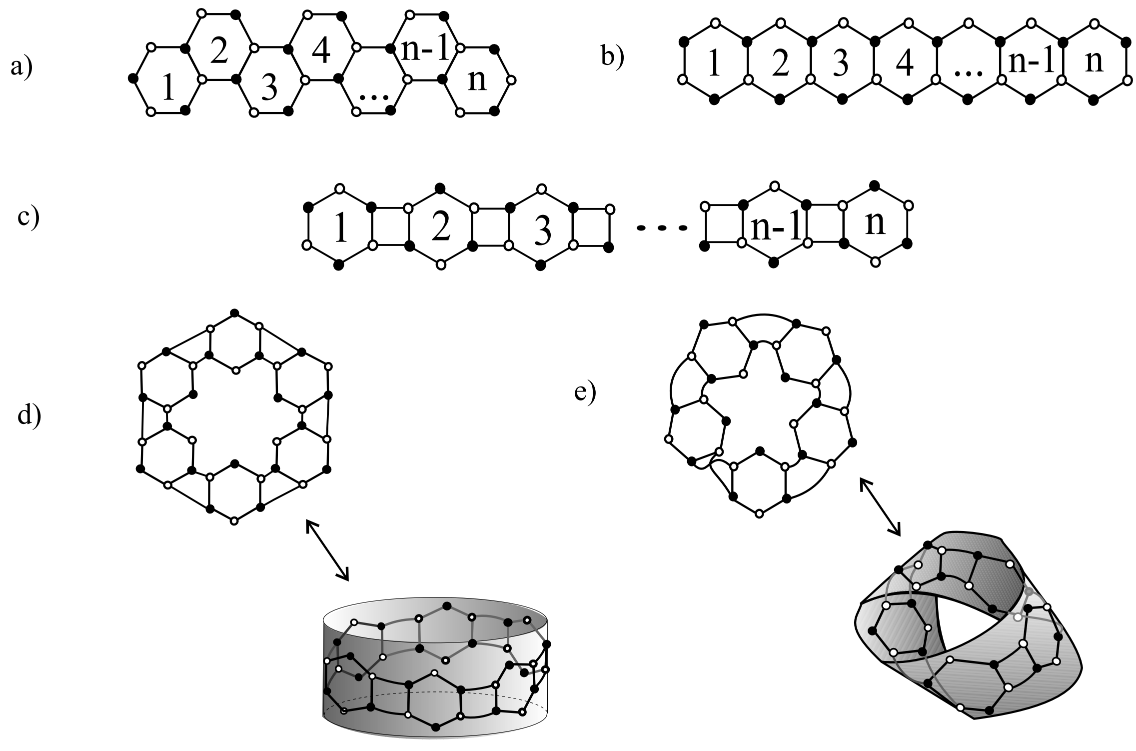

Fig. 1 : a) The zig-zag chain of n hexagons; b) The linear chain of n hexagons (The structure of the linear polyacenes); c) The open linear hexagonal-square chain (The structure of the linear phenylenes); d) The closed linear hexagonal-square chain (planar); e) The closed linear hexagonal-square chain (non-planar)

In the case of non-benzenoid bipartite graphs (in which some cells are circuits of length of the form $4s, \;\; s = 1, 2, \ldots$) these two numbers $ASC\{G\}$ and $K\{G\}$ are usually different. For example, the ASC-value and K-value of the graph depicted in Fig. 1c) (Linear [n]-phenylene) are equal to $n+1$ and $(1-\sqrt{2})^n(2-\sqrt{2})/4 + (1+\sqrt{2})^n(2+\sqrt{2})/4$ respectively, and the ASC-values for the graphs depicted in Fig. 1d) and Fig. 1e) are equal to zero. Angular hexagonal-square chains (open and closed) belong to this class of graphs.

Definition 1.
The open (closed) angular hexagonal-square chain O_n (C_n) *is a connected, bipartite, plane graph which consists of* n *hexagons linearly (cyclically) concatenated by circuits of length* 4 *which we call squares in the following way. For each* $i = 1, 2, \ldots, n-1$ $(i = 1, 2, \ldots, n)$, *the square* α_i *connects two hexagons* H_i *and* H_{i+1} *(subscripts are taken modulo n) and for each* $i = 2, \ldots, n-1$ $(i = 1, \ldots, n)$, *there exists an edge of* H_i *joining two vertices of squares* α_{i-1} *and* α_i $(\alpha_0 \stackrel{def}{=} \alpha_n)$.

Fig. 2a) and 2b) show some of the possible open and closed angular hexagonal-square chains, respectively. Note that in the case of the graph C_n there exist two face-boundaries which are different from squares and hexagons (one of these regions is infinite). We call them *external circuits.* In the case of the graph O_n there is only one *external circuit* which is the boundary of the infinite region.

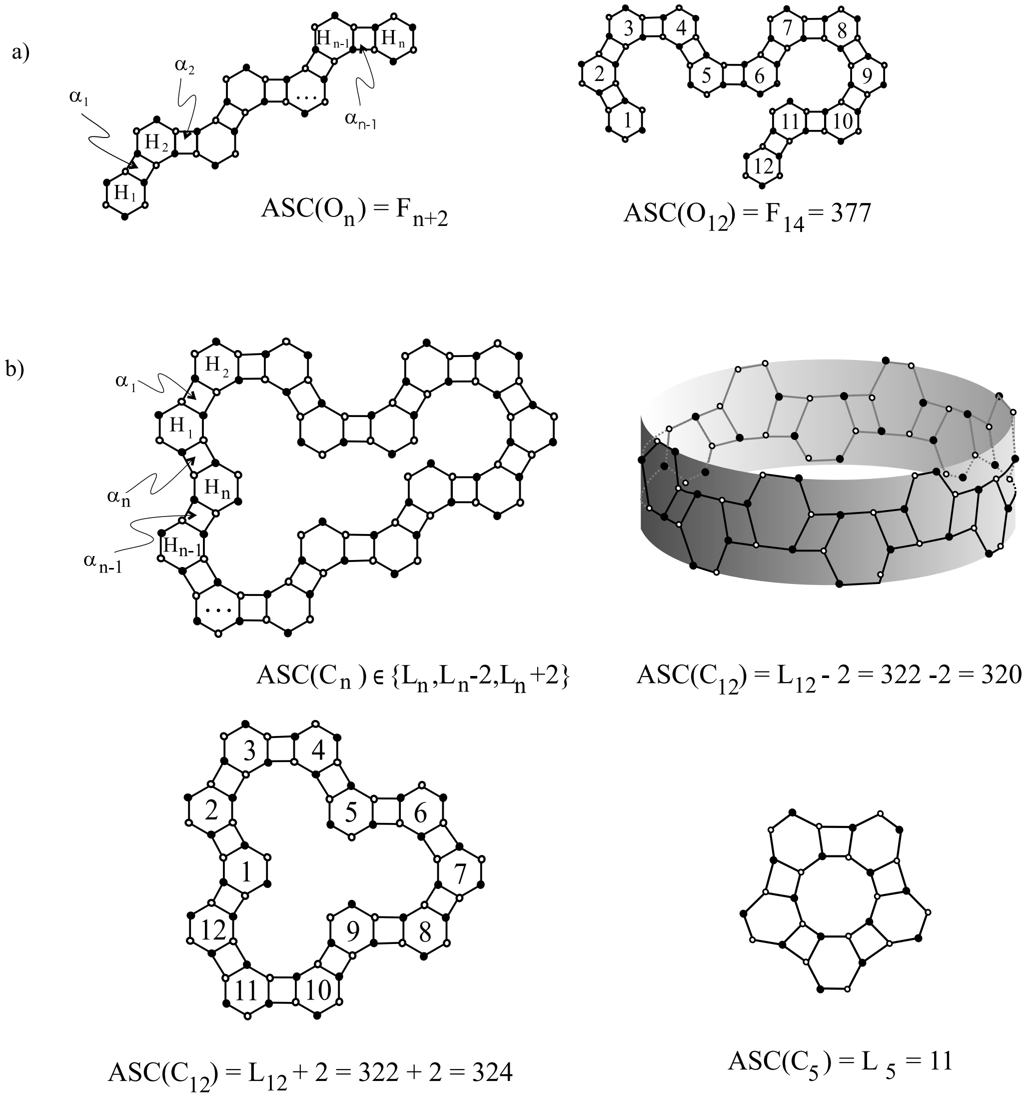

Fig. 2 : a) The open angular hexagonal-square chains; b) The closed angular hexagonal-square chains

The aim of this paper is to prove the following two statements.

Theorem 1.

$$ASC\{O_n\} = F_{n+2} \ ,$$

where F_n *is the* n^{th} *Fibonacci number.*

Theorem 2.

$$ASC\{C_n\} = \begin{cases} L_n, & if \;\; n \;\; is \; odd \; ; \\ L_n - 2, & if \;\; n \;\; is \; even \; and \;\; c \equiv 0(mod 4); \\ L_n + 2, & if \;\; n \;\; is \; even \; and \;\; c \equiv 2(mod 4); \end{cases}$$

where c is the length of one of two boundary circuits and L_n is the n^{th} Lucas number.

Actually, Theorem 1 has been known for a long time [?] and can be deduced as a special case of the result obtained for a class of non-benzenoid hydrocarbons which we already reported in [?]. Now, we deduce the theorem using some simple enumeration arguments. Continuing in the same manner we obtain the new result of Theorem 2.

2 Preliminaries

Let G be a connected, plane bipartite graph with $n+n$ vertices - graph whose all circuits are of even length. Define a binary relation ρ in the set of all perfect matchings of G in the following way:

Two perfect matchings P_1 and P_2 are in relation ρ iff the union of the sets of edges of P_1 and P_2 forms an even number of circuits of length $4s$ $(s = 1, 2, \ldots)$.

It can be proved that this binary relation is an equivalence relation and subdivides the set of perfect matchings into two equivalence classes [?]. In [?] this relation is called "being of the same parity" and the numbers of these classes are denoted by K_+ and K_-. The theorem by Dewar and Longuet-Higgins [?] yields the following corollary

$$ASC\{G\} = \mid K_+ - K_- \mid . \tag{1}$$

From the definition of the relation ρ it follows that two perfect matchings are in distinct classes (of opposite parity) if one is obtained from the other by cyclically rearranging an even number edges within a single circuit. If the number of cyclically rearranged double bonds is odd, then the respective two perfect matchings are of equal parity.

Consider a perfect matching of O_n or C_n. Note that edges belonging to the perfect matching can be arranged in and around a square in seven different ways (*modes* 1-7), as it is shown in Fig.3 (these edges are marked by double lines). In the case of the graph C_n the position of the observer is in the finite region determined by an external circuit.

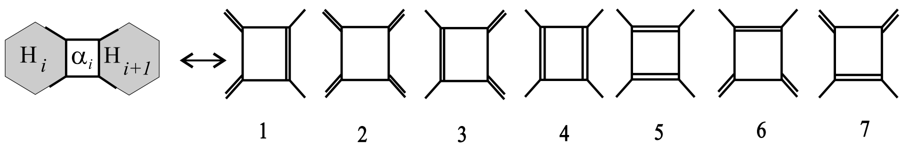

Fig. 3: The seven modes in which double bonds can be arranged in and around a square

Definition 2. *The arrangement word of a perfect matching of the graph O_n (C_n) is the word $u = u_1u_2 \ldots u_{n-1}$ $(u = u_1u_2 \ldots u_n)$ from the set $\{1, 2, \ldots, 6, 7\}^{n-1}$ $(\{1, 2, \ldots, 6, 7\}^n)$, where u_i is the mode (1-7) of the arrangement of edges of the perfect matching in and around the square α_i for $i = 1, \ldots, n-1$ $(i = 1, \ldots, n)$.*

For example, the arrangement words of the perfect matchings, which are represented in Fig. 4, are $u = 21322$, 21432, 21532, 77777 and 66666, respectively. Note that the modes 4 and 5 (Fig. 4b and Fig. 4c) are interconverted by rearranging two (an even number) edges. Therefore, modes 4 and 5 are of opposite parity. It implies that the perfect matchings in which they appear can be excluded from consideration when the algebraic structure count is evaluated. For the purpose of evaluation ASC-values for O_n and C_n, introduce the so-called "good" perfect matchings.

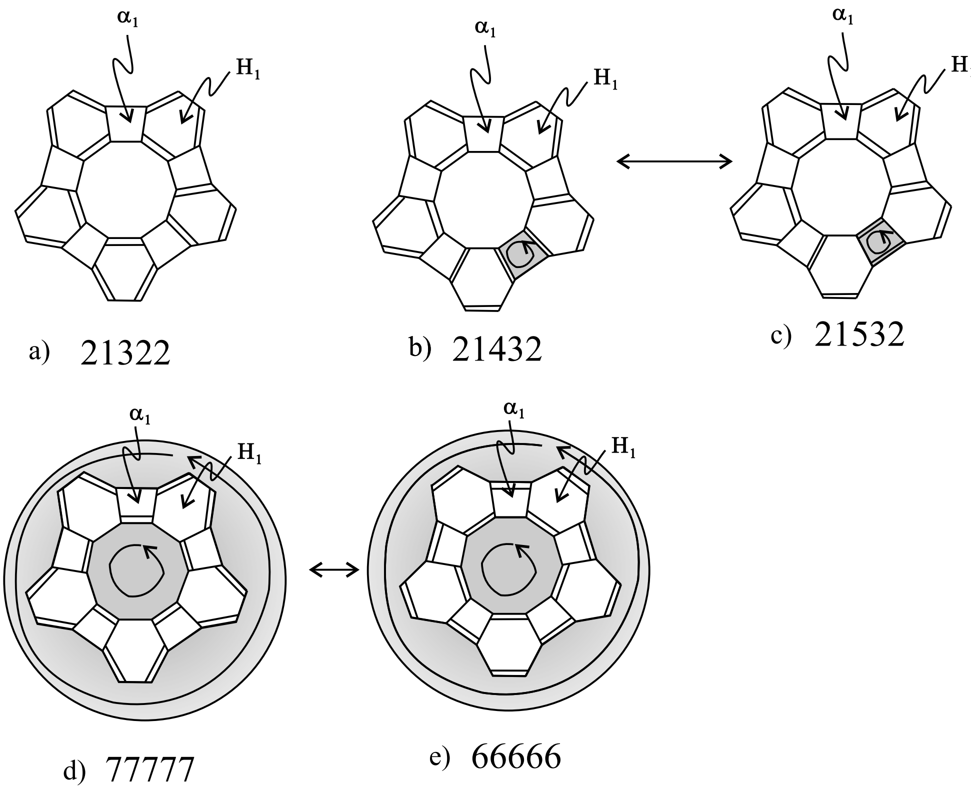

Fig. 4: Some of possible perfect matchings for C_5 with their arrangement words.
Rearranging two edges in the perfect matching represented in b) we obtain the one represented in c). If we cyclically rearrange the edges of the perfect matching represented in d) within one of the external circuits first, and then within the other one, we obtain the perfect matching represented in e).

Definition 3. *The perfect matchings are called good if their arrangement words belong to the set* $\{1, 2, 3\}^n$.

Note that the edges of squares belonging to boundary circuits of C_n or O_n (horizontal lines in Fig.3) are never in any good perfect matching. This means that every good perfect matching of the graph C_n or O_n induces a perfect matching in every hexagon H_i i.e. the edges of the good perfect matching can be rearranged only within each fragment H_i. Consequently, all good perfect matchings are of equal parity. Next, the modes 6 and 7 are impossible to appear in the arrangement word of a perfect matching of O_n because there are an even number of vertices appearing on every side of an arbitrary square of O_n. This implies that $ASC(O_n)$ is equal to the number of all good perfect matchings. In the case of the graph C_n there are exactly two perfect matchings whose arrangement words contain at least one of numbers from the set $\{6, 7\}$. Note that their arrangement words must be the words $77\ldots7$ and $66\ldots6$ (Fig. 4d and Fig. 4e) because an appearance of the number 6 or 7 as a mode for a square implies appearances the same number as modes for adjacent squares.

3 Proof of Theorem 1

In order to obtain the number of all good perfect matchings for the graph O_n observe one of its good perfect matchings and edges of the perfect matching belonging to the hexagon H_i $(2 \leq i \leq n-1)$. The hexagon H_i $(2 \leq i \leq n-1)$ and its adjacent squares α_{i-1} and α_i have two edges in common. Either both of them belong to the good perfect matching or neither of them do.

Now, associate with each good perfect matching of O_n a word $h_1h_2\ldots h_n$ on the alphabet

$\{0,1\}$ in the following way: If in the set of edges of H_i belonging to the perfect matching there exists an edge of an adjacent square, then $h_i = 0$; otherwise $h_i = 1$. So, from our observation above we obtain that $ASC(O_n) = F_{n+2}$, because this is the number of words in $\{0,1\}^n$ with forbidden subword 00 [?].

□

4 Proof of Theorem 2

In order to obtain the number of all good perfect matchings for the graph C_n, adopt the same definition of the mapping which associates with each good perfect matching of C_n a word $h_1h_2\dots h_n$ on the alphabet $\{0,1\}$ as we have done for the case O_n. In this case the number of all good perfect matchings for the graph C_n is equal to $g(n)$, where $g(n)$ is the number of words in $\{0,1\}^n$ with forbidden subword 00 and for which $h_1h_n \neq 00$, so $g(n) = L_n$ [?].

On the other hand, there are two perfect matchings whose arrangement words contain at least one of numbers from the set $\{6,7\}$. Recall that their arrangement words are $77\dots7$ and $66\dots6$.

If n is odd, then the length of one of the external circuits is $\equiv 0(mod4)$ and the length of the other one is $\equiv 2(mod4)$. If we cyclically rearrange the edges of one of these perfect matchings within one of the external circuits first, and then within the other one, we obtain the other perfect matching (Fig. 4d and Fig. 4e). This implies that these two perfect matchings are of opposite parity, so $ASC(C_n) = g(n) = L_n$.

If n is even, then the lengths of external circuits are both $\equiv 0(mod4)$ or $\equiv 2(mod4)$. In this case these two perfect matchings are of equal parity. Observe the perfect matching with the arrangement word $77\dots7$ and the external circuit which is boundary of the finite region. Let the length of the circuit be denoted by c. If we cyclically rearrange the edges of the considered perfect matching within the observed external circuit, we obtain one of the good perfect matchings. So, if $c \equiv 0(mod4)$ (we have rearranged an even number of edges), then the perfect matchings corresponding to the arrangement words $66\dots$ and $77\dots7$ are of equal parity, opposite to the parity of good perfect matchings. In this case we have $ASC(C_n) = g(n) - 2 = L_n - 2$.

In the other case, if $c \equiv 2(mod4)$ (we have rearranged an odd number of edges), then the perfect matchings corresponding to the arrangement words $66\dots$ and $77\dots7$ are of equal parity, equal to the parity of good perfect matchings. In this case we have $ASC(C_n) = g(n) + 2 = L_n + 2$.

□

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