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Note

Kekulé structures of square–hexagonal chains and the Hosoya index of caterpillar trees

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ABSTRACT

Let R_n be a square–hexagonal chain. In this paper, we show that there exists a caterpillar tree T_n such that the number of Kekulé structures of R_n is equal to the Hosoya index of T_n. Since both hexagonal chains and polyomino chains can be viewed as special square–hexagonal chains, our result generalizes the corresponding results for hexagonal chains (Gutman, 1977) and polyomino chains (Liand Yan, 2012).

1. Introduction

Let $G = (V, E)$ be a molecule graph. Denote by $m(G, k)$ the number of ways in which k mutually independent edges can be selected in G, set $m(G, 0) = 1$ by convention. Thus $m(G, 1)$ is equal to the number of edges of G. If n is even, then $m(G, \frac{n}{2})$ is the number of *Kekulé structures* (or *perfect matchings*) of G and will be denoted by $M(G)$. The number of matchings of G is called the *Hosoya index* [7] and will be denoted by $Z(G)$. That is

$$Z(G) = m(G, 0) + m(G, 1) + \cdots + m\left(G, \left[\frac{n}{2}\right]\right).$$

By a square–hexagonal chain R_n, we mean a finite graph obtained by concatenating n cells (where each cell can be either a square or a hexagon) in such a way that any two adjacent cells have exactly one edge in common, and each cell is adjacent to exactly two other cells, except the first and last cells (end cells) which are adjacent to exactly one other cell each (see an illustration example with ten cells in Fig. 1(a)). It is clear that different square–hexagonal chains will result, not only according to the manner in which the cells are concatenated, but also the cell's type. For example, we have hexagonal chains if all the cells are hexagons, and we have polyomino chains if all the cells are squares. Similarly, we have phenylene chains if hexagons and squares are concatenated alternately.

In 1977 Gutman [4] discovered a curious relation between the sextet polynomial of a hexagonal chain and the matching polynomial of a caterpillar tree (so this tree is also named as Gutman tree by some researchers, see [1,2] for example). This result implied that, for a hexagonal chain H, there exists a corresponding caterpillar tree T such that the number of Kekulé structures of H is equal to the Hosoya index of T. Some related results see for example [5,8,11]. More recently, Li and Yan in [9] proved a similar result for polyomino chains. In this paper, we will show that, for a general square–hexagonal chain R_n, there exists a corresponding caterpillar tree T_n such that the number of Kekulé structures of R_n is equal to the Hosoya index of T_n. So our result includes Gutman, Li and Yan's results mentioned above as special cases.

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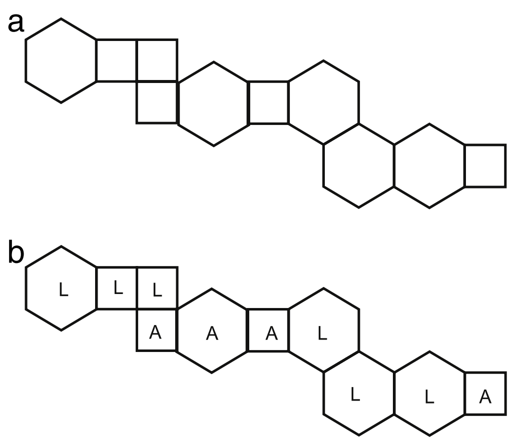

Fig. 1. (a) A square–hexagonal chain R_n with 10 cells. (b) The *LA*-sequence of R_n is *LLLAAALLLA*.

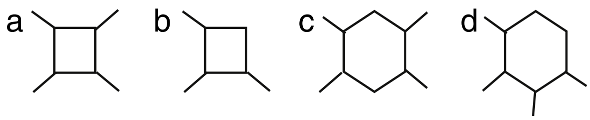

Fig. 2. Concatenation modes of cells that occur in square–hexagonal chains.

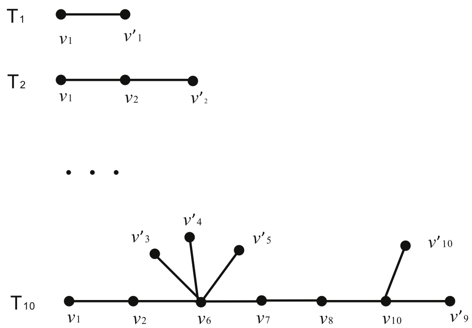

Fig. 3. The recursive construction of tree T_{10} corresponding to R_{10} in Fig. 1.

As in [4] and [9], we will prove our result by first constructing a caterpillar tree T_n explicitly for any given square–hexagonal chain R_n, then showing that $M(R_n) = Z(T_n)$. But the constructing method that we give below is recursive, while none of the constructions in [4] and [9] is. We will explain more clearly in the remarks.

Now for a square–hexagonal chain R_n with n cells $c_1, c_2, \ldots, c_n$, where the cells are numbered successively. That is, the cell c_i $(1 < i < n)$ is neighbouring to the cells c_{i-1} and c_{i+1}. Then it is easy to see that a cell in R_n with exactly two neighbours is concatenated in one of the four modes: a, b, c, d (see Fig. 2). We define a function f from the cells to the symbols L and A as follows:

$$f(c_i) = \begin{cases} L, & i = 1, 2; \\ L, & \text{if } i \geq 3 \text{ and the concatenating mode of } c_{i-1} \text{ is ``}a\text{'' or ``}d\text{''}; \\ A, & \text{otherwise.} \end{cases}$$

Thus a unique *LA*-sequence $f(c_1)f(c_2)\cdots f(c_n)$ is associated with R_n (see Fig. 1(b) for an example). Note that if let R_i $(1 \leq i \leq n)$ denote the subchain of R_n with the first i cells, then the corresponding *LA*-sequence of R_i is just the subsequence $f(c_1)f(c_2)\cdots f(c_i)$. So we can construct a caterpillar tree T_n corresponding to R_n recursively as follows.

First let $T_1 = P_2$ with two vertices labelled by v_1 and v_1' respectively (see Fig. 3). Now suppose we have constructed T_i corresponding to R_i, then T_{i+1} is obtained from T_i by attaching a new edge e_{i+1} to the vertex v_i' or v_i of T_i according to $f(c_{i+1}) = L$ or A. At the same time, the labelling of the attaching vertex is changed to v_{i+1}, the other end vertex of e_{i+1} is labelled as v_{i+1}'. The caterpillar tree corresponding to the square–hexagonal chain in Fig. 1 is shown in Fig. 3.

In the next section, we shall show that the number of Kekulé structures of R_n is equal to the Hosoya index of T_n.