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The anti-forcing number of hexagonal chains[1]

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Abstract

The anti-forcing number is the smallest number of edges that have to be removed that any benzenoid remains with a single Kekulé structure. In this paper, we give a algorithm for computing the anti-forcing number of hexagonal chains and determine the bounds of the anti-forcing number of hexagonal chains.

1 Introduction

The connection between graph theory and chemistry is very important. Especially, the concept of perfect matchings from graph theory is related to study of benzenoids. The perfect matchings or the Kekulé structures later attracted considerable interest in graph theory and chemistry

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The forcing number of benzenoids was introduced by Harary et al. [1] in 1991. The roots of this concept can be found in an earlier paper by Randić and Klein [2]. There, the forcing number has been called the innate degree of freedom of a Kekulé structure, although the term the forcing number was also used. The forcing number is equal to the smallest number of double bonds that completely determine the Kekulé structure of a given benzenoid. After this initial report, several papers appeared reporting the forcing number of hexagonal systems and square grids [3,4].

Later, Došlić [5] introduced the global forcing number of a graph and gave several results concerning global forcing sets and numbers of benzenoid graphs. In particular, he proved that all catacondensed benzenoids and catafused coronoids with n hexagons have the global forcing number equal to n, and that for pericondensed benzenoids the global forcing number is always strictly smaller than the number of hexagons.

Recently, Vukičević and Trinajstić [6] introduced the anti-forcing number as the smallest number of edges that have to be removed from a benzenoid to remain with a single Kekulé structure, and determined the anti-forcing number of benzenoid parallelograms.

In this paper, we will determine the anti-forcing number of any hexagonal chain.

2 The definition of anti-forcing set

All graphs in this paper are simple, connected, and have a perfect matching, if not explicitly stated otherwise. For all terms and notation not defined here we refer the reader to [7]. A perfect matching in a graph G is a set M of edges of G such that every vertex of G is incident with exactly one edge from M.

Let $G = (V, E)$ be a graph G with a perfect matching. An anti-forcing set of G is a subset A of E such that $G - A$ has a unique Kekulé structure. An anti-forcing set of the smallest cardinality is called a minimal anti-forcing set, and its cardinality is the anti-forcing number of G and it is denoted by $af(G)$ (see [6]).

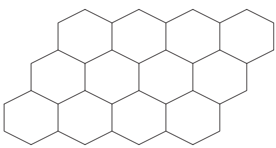


Figure 1. $B_{3,4}$

In [6], the minimal anti-forcing set and the anti-forcing number of the benzenoid parallelogram [8-10] $B_{m,n}$ are determined, where $B_{m,n}$ is consisting of $m \times n$ hexagons, arranged in m rows, each row consisting of n hexagons, $af(B_{m,n}) = 1$.

3 The anti-forcing number of hexagonal chains

Let us now consider the main subject of the present paper, the hexagonal chains. Hexagonal systems are of great importance for theoretical chemistry because they are the molecular graphs (or, more precisely, the graphs representing the carbon-atom skeleton) of benzenoid hydrocarbons. The mathematical theory of hexagonal systems is nowadays being greatly expanded.

Our standard reference for any terminology of hexagonal systems is [11].

A hexagonal system [11] is a connected plane graph without cut-vertices in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge.

The hexagonal systems are divided [11] into catacondensed and pericondensed hexagonal systems. In a pericondensed hexagonal system there exist three hexagons sharing a common vertex; In catacondensed hexagonal systems no three hexagons share a common vertex.

Catacondensed hexagonal systems are further classified into non-branched (in which no hexagon has more than two neighboring hexagons) and branched (in which at least one hexagon has three neighboring hexagons). A catacondensed hexagonal system without branched hexagons is called a hexagonal chain. Each hexagon in a hexagonal chain is adjacent to at most two hexagons.

A hexagonal chain with h hexagons, $h > 2$, possesses two terminal hexagons and $h - 2$ hexagons that have two neighbors. Hexagons being adjacent to exactly two other hexagons are classified as angularly or linearly adhesive. A hexagon adjacent to exactly two other hexagons possesses two vertices of degree 2. If these two vertices are adjacent, then the hexagon is angularly adhesive, if these two vertices are not adjacent, then it is linearly adhesive.

A linear chain L_h with h hexagons is a hexagonal chain without any angularly adhesion (see Figure 2).

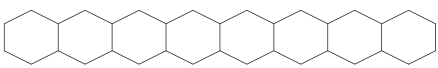


Figure 2. The linear chain L_8.

A fibonacene chain is a hexagonal chain without linearly adhesive hexagons (see Figure 3).

One should note that fibonacene chains may be helical or jammed.

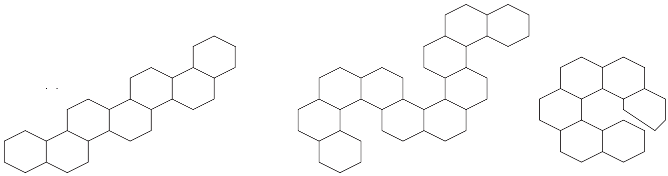


Figure 2. Some fibonacene chains.

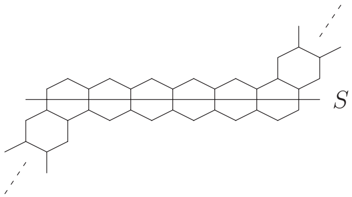


Figure 4. A segment S with length 6 in a hexagonal chain.

A segment [11,12] is a maximal linear chain in a hexagonal chain, including the angularly adhesive hexagons and/or terminal hexagons at its end. The number of hexagons in a segment S is called its length and is denoted by $l(S)$. For any segment S of a hexagonal chain with h hexagons, $2 \leq l(S) \leq h$. Particularly, a hexagonal chain is a fibonacene chain if and only if the lengths of its segment are all equal to 2 and a hexagonal chain is a linear chain if and only if the length of its unique segment is h.

Lemma 1. Let $G = (V, E)$ be a hexagonal chain. If A is an anti-forcing set of G. Then, for any hexagon H in G, at least one edge on the segment containing H belongs to A.

Proof. By contradiction, we assume that there is a hexagon H_0 of G such that the segment S_0 containing H_0 has no edge in A. Let l_0 be the length of S_0 and M the unique perfect matching of $G - A$.

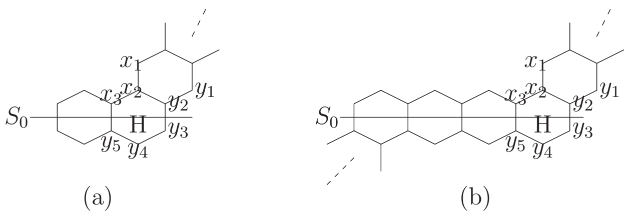


Figure 5.

(I) If $l_0 = 2$ and S_0 is at the end of the hexagonal chain G, or $l_0 > 2$, see Figure 5(a) or (b), then either both x_2x_3 and y_2y_3 are in M, or none edge of them is in M.

(i) If both x_2x_3 and y_2y_3 are in M, then $y_4y_5 \in M$, and H is an M-alternating circuit, $G - A$ has at least two perfect matchings.

(ii) If no edge of x_2x_3 and y_2y_3 is in M, then $y_4y_5 \notin M$, $y_3y_4 \in M$. And $S_0 - \{x_2, y_3, y_4\}$ contains an M-alternating circuit, $G - A$ has at least two perfect matchings.

(II) If $l_0 = 2$ and S_0 is not at the end of the hexagonal chain G, see Figure 6, then both x_2x_3 and y_2y_3 are in M, or no edge of x_2x_3 and y_2y_3 is in M, and S_1 has no edge of A.

(i) If both x_2x_3 and y_2y_3 are in M, then H_1 is a M-alternating circuit, and $G - A$ has at least two perfect matchings.

(ii) If no edge of x_2x_3 and y_2y_3 is in M, then $y_3y_4 \in M$, $y_4y_5 \notin M$. And there is a M-alternating circuit in S_1, $G - A$ has at least two perfect matchings.

Therefore, the result holds.

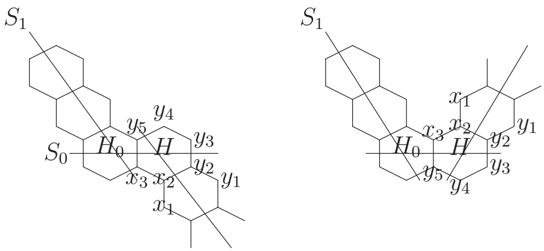


Figure 6.

Now we introduce a new concept. The figure consisting of two adjacent segments in a hexagonal chain G is called a broken line, and the edge crossed by the bisector of the $240°$ angle is called a broken edge (see Figure 7).

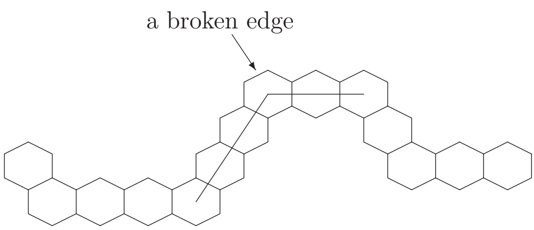
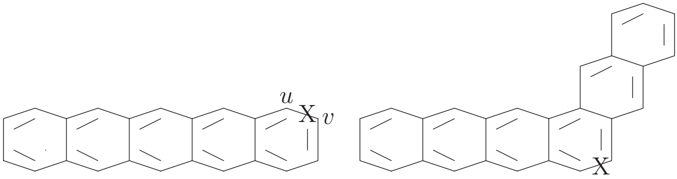


Figure 7. A broken line and a broken edge in a hexagonal chain.

Remark. If we delete the broken edge in a broken line or the slant edge incident with two vertices of degree 2 in a linear chain, then there is only one perfect matching (see Figure 8).



(a) (b)

Figure 8.

If there is an edge e of a hexagonal chain G such that the perfect matching of a hexagon H is unique after deleting e, then we say that e dominates the hexagon H. Let A be any anti-forcing set of G. From Lemma 1, we need at least one edge of A for dominating the hexagons on S for each segment S of G.

The following algorithm will give a minimal anti-forcing set and the anti-forcing number $af(G)$ of a hexagonal chain G.

Algorithm

Let G be a hexagonal chain. u, v are two adjacent vertices with degree 2 on the last hexagon of G such that the degree of the other vertex adjacent to u is 3. When a hexagon is deleted from a hexagonal chain, the common edges of the hexagon and its neighboring hexagons are left. Let $A = \emptyset$.

If G is a linear chain, then $A \leftarrow A \cup \{uv\}$ and stop.

If G is not a linear chain, then

(i)Let L be the first broken line and e the broken edge of L, and $A \leftarrow A \cup \{e\}$, $G \leftarrow G - L$;

(ii)If G is neither empty nor a linear chain, then return to (i);

(iii)If G is empty, then stop;

(iv)If G is a linear chain, then $A \leftarrow A \cup \{uv\}$ and stop.

Theorem 2. The set A given by the algorithm above is a minimal anti-forcing set of G.

Proof. By the remark above, A is a anti-forcing set of G.

Now, we prove that the set A is a minimal anti-forcing set of G by using Lemma 1.

If G is a linear chain or a broken line, then the result is true since $af(G) \geq 1$ (also see Figure 8).

Let G be the hexagonal chain. $L_1, L_2, \cdots, L_k$ are the broken lines of G deleted in the algorithm. $s_1, s_2, \cdots, s_{2k}$ are the segments such that $L_1 = s_1 \cup s_2$ and $L_i = s_{2i-1} \cup s_{2i} - s_{2i-2}$, $i = 2, 3, \cdots, k$. Then the length of s_{2i-1} is at least 3 if s_{2i-1} and s_{2i-2} have a common hexagon from the algorithm.

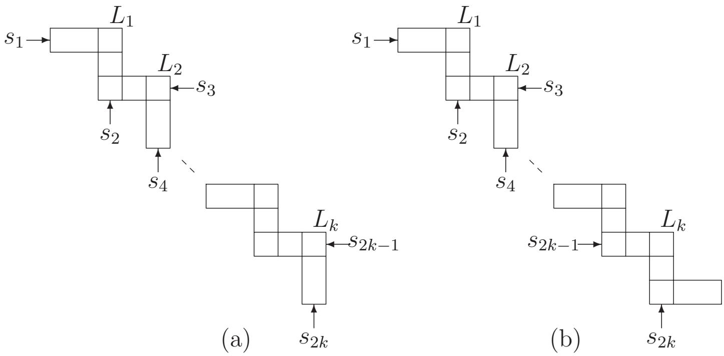
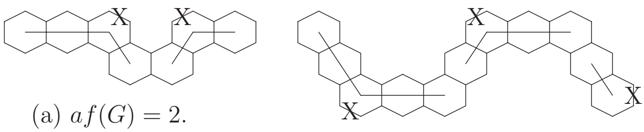


Figure 10.

If G is empty after deleting $L_1, L_2, \cdots, L_k$ from G (see Figure 10(a)), then $|A| = k$. So, there does not exist an edge e such that e can dominate the hexagons on both s_{2i-1} and s_{2j-1}, $i \neq j$. By Lemma 1, any anti-forcing set of G must contain k edges. Therefore, A is a minimal anti-forcing set.

If G is a linear chain after deleting $L_1, L_2, \cdots, L_k$ from G (see Figure 10(b)), then $|A| = k+1$, and at least one edge is needed for dominating the hexagons of $G - L_1 \cup L_2 \cup \cdots \cup L_k$. But no edge can dominate the hexagons on both s_{2i-1} and s_{2j-1}, $1 \leq i < j \leq k$. By Lemma 1, any anti-forcing set of G must contain $k+1$ edges. Therefore, A is a minimal anti-forcing set.

Example. Using the algorithm above, we can easily obtain the anti-forcing numbers of the hexagonal chains in Figure 9.



(a) $af(G) = 2$.

(b) $af(G) = 3$.

Figure 9.

The following results are immediate from the algorithm.

Corollary 3. If the number of segments in a hexagonal chain G is s, then $af(G) \leq \frac{s+1}{2}$.

Corollary 4. Let F_n be a fibonacene chain with n hexagons. Then $af(F_n) = \lceil \frac{n}{3} \rceil$, where $\lceil x \rceil$ is the minimal integer not less than x.

Corollary 5. Let G be a hexagonal chain with n hexagons. If G is neither a linear chain L_n nor a fibonacene chain F_n, then

$$1 = af(L_n) < af(G) < af(F_n) = \lceil \frac{n}{3} \rceil.$$

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