Journal of Mathematical Chemistry Vol. 38, No. 4, November 2005 (© 2005)
DOI: 10.1007/s10910-005-6915-1

Perfect matchings in bipartite lattice animals: Lower bounds and realizability

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Received 28 April 2005; revised 27 May 2005

In the first part of this paper we establish sharp lower bounds on the number of perfect matchings in benzenoid graphs and polyominoes. The results are then used to determine which integers can appear as the number of perfect matchings of infinitely many benzenoids and/or polyominoes. Finally, we consider the problem of concealed non-Kekuléan polyominoes. It is shown that the smallest such polyomino has 15 squares, and that such polyominoes on n squares exist for all $n \geqslant 15$.

KEY WORDS: lattice animal, benzenoid graph, polyomino, perfect matching, lower bound, realizability

MSC: 05C70, 05A15, 92E10

1. Introduction

In this article we take further the line of research developed in a series of recent papers on perfect matchings in plane bipartite graphs [1,2,3]. Common to all three papers is the application of the structural theory of matchings [4] to some problems concerning the structure and the enumeration of perfect matching in such graphs. Here we restrict our attention to bipartite lattice animals, i.e., to the polyhexes and polyominoes, and show how the structural results from [1] can be used to obtain sharp lower bounds on the number of perfect matchings in these two classes of graphs. Then we proceed by using these results to answer the question whether, for a given positive integer n, there are finitely or infinitely many benzenoids (or polyominoes) with n perfect matchings. The case $n = 0$ is discussed in more detail, and the paper is concluded by presenting the smallest concealed non-Kekuléan polyomino.

2. Definitions and preliminaries

A **lattice animal** is a 1-connected collection of congruent regular polygons arranged in a plane in such a way that the interior of the collection is

1-connected, and any two polygons that intersect in more than one point intersect in a whole edge. From the conditions of regularity and congruence of the basic polygons it follows that the lattice animals are subsets (with 1-connected interior) of regular tilings of the plane. The three different regular tilings give rise to three different classes of lattice animals. Here we consider only two of these three classes, those consisting of squares (known as **polyominoes**), and those consisting of regular hexagons (known also as **polyhexes** or **benzenoid systems**).

To each lattice animal we assign a graph by taking the vertices of polygons as the vertices of the graph, and the sides of polygons as the edges of the graph. The resulting **animal graph** is simple, plane, and bipartite. (We refer the reader to any standard textbook, such as [5] or [6], for the graph-theoretic terms and concepts not defined here.) The vertices lying on the border of the unbounded face of an animal graph are called **external**; other vertices, if present, are called **internal**. An animal graph without internal vertices is **catacondensed**. Otherwise, the graph is **pericondensed**. In the rest of this paper when referring to lattice animals we will be referring to the corresponding animal graphs.

A **perfect matching** in a graph G is a collection M of edges of G such that every vertex of G is incident with exactly one edge from M. An edge e of G is **allowed** if it appears in some perfect matching of G; otherwise, the edge is **forbidden**. A graph G is **elementary** if its allowed edges form a connected subgraph of G. In chemical literature the elementary graphs, especially elementary benzenoids, are also called **normal**. For connected bipartite graphs, the elementarity is equivalent to the property that all edges are allowed ([4], p. 122).

Perfect matchings in benzenoid graphs are known in chemical literature as **Kekulé structures**, and the benzenoids possessing them are called **Kekuléan**. The literature on the subject of enumeration of perfect matchings in benzenoids is vast. For a review, the reader might wish to see, e.g., [7] or [8] and the references therein. These references contain a wealth of exact results valid for particular classes of benzenoid graphs. Here we are concerned with different type of results: we are trying to establish lower bounds on the number of perfect matchings that will be valid across the whole spectrum of benzenoid and polyomino graphs.

For normal (i.e. elementary) bipartite lattice animals the question was settled in reference [3].

Theorem A. In a normal bipartite lattice animal with h basic polygons there are at least $h + 1$ different perfect matchings. □

The lower bound of Theorem A is sharp. It can be easily seen that the lattice animals with h basic polygons shown in figure 1 are normal and have exactly $h + 1$ different perfect matchings.

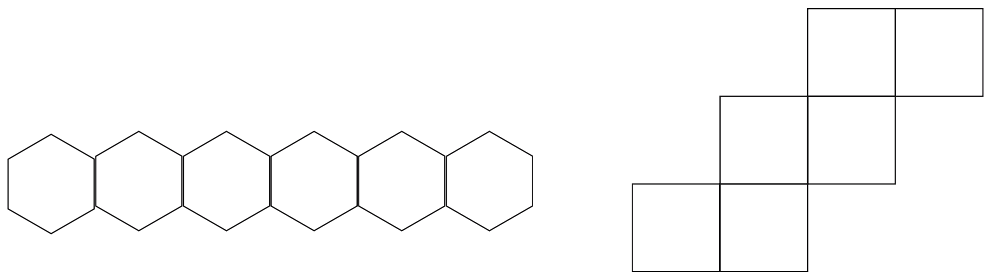

Figure 1. Extermal lattice animals with respect to the number of perfect matchings.

An immediate consequence of Theorem A is that, for a given positive integer n, there are finitely many normal bipartite lattice animals with exactly n (or with at most n) perfect matchings.

Let us now consider the lattice animals with perfect matchings that are not normal. In the benzenoid context such graphs are called **essentially disconnected**, and we extend the terminology also to the case of polyominoes. The name is justified by the fact that removal of forbidden edges from such a graph results in a disconnected collection of normal components. If all faces of a normal component of a graph G are also faces of G, the normal component is called a **normal block**. It can be shown [1] that all normal components of essentially disconnected lattice animals are indeed normal blocks. The following two results from the same reference will be essential for establishing lower bounds on the number of perfect matchings in non-normal bipartite lattice animals. We quote them in a slightly more general terms than needed in this paper, so we leave out the precise definition of weakly elementary graphs. It suffices to know that the class is wide enough to encompass plane bipartite graphs, and hence also the bipartite lattice animals [1].

Theorem B. Let a graph G be weakly elementary, without vertices of degree one. If G has a forbidden edge, then G has at least two normal blocks. □

Theorem C. Let a graph G be 2-connected and weakly elementary. Assume that G has more than one cycle and all vertices of degree 2 lie on the boundary of G. If G has $m \geqslant 1$ distinct cycles as normal blocks, then G has $m + 2$ normal blocks. □

3. Lower bounds

The lower bounds we are seeking to establish follow from Theorems B and C and the fact that the number of perfect matchings in a non-elementary graph is equal to the product of numbers of perfect matchings of its normal components.

Theorem 1. Let G be an essentially disconnected benzenoid graph with a perfect matching. Then G has at least 9 different perfect matchings.

Proof. According to Theorem B, G has at least two normal blocks. If none of these is a single hexagon, then each of them must have at least three different perfect matchings, and the claim of the theorem follows. If there are m normal blocks that are single hexagons, Theorem C gives us the existence of at least two normal blocks with more than one hexagon, and the minimal number of different perfect matchings in G is at least $2^m \cdot 3^2$. □

By merging Theorem A and Theorem 1 we obtain the following result.

Corollary 2. Let G be a benzenoid graph with a perfect matching and at least 8 hexagons. Then G has at least 9 different perfect matchings.

Proof. If G is normal, the claim follows from Theorem A; otherwise, it follows from Theorem 1. □

The lower bound of Theorem 1 is the best possible, since for all $h \geqslant 5$ there are Kekuléan benzenoids with h hexagons and exactly 9 perfect matchings. An example of such a graph is shown in figure 2.

Hence, the list of Kekuléan benzenoids with less than 9 perfect matchings is finite and indeed short.

The case of polyominoes is a bit more complicated. The simplest normal polyomino that is not a single square is a domino consisting of two squares that share a side. We first show that among the normal blocks of an essentially disconnected polyomino must be at least two that are neither a single square nor a domino. We call such a normal block **proper**.

Lemma 3. An essentially disconnected polyomino has at least two proper normal blocks.

Proof. Let G be an essentially disconnected polyomino with k_1 single squares and k_2 dominoes as normal blocks. By deleting the edge common to both squares in each domino normal block, we obtain a graph G' that satisfies the

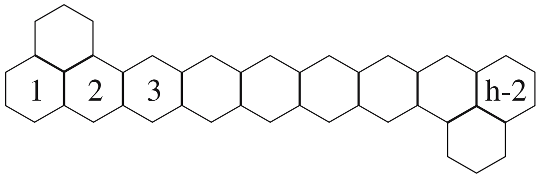

Figure 2. A benzenoid with h hexagons and only 9 perfect matchings.

conditions of Theorem C and that has $k_1 + k_2$ single cycles as normal blocks. Hence, G' must have at least two normal blocks that are neither single squares nor dominoes. From construction of G' it follows that all its normal blocks are also normal blocks of G, and that the number of perfect matchings in G' does not exceed the number of perfect matchings in G. □

That the domino graph can appear as a normal block of an essentially disconnected polyomino can be seen from the example shown in figure 3.

Let us pause here for a moment and comment on a difference between polyominoes and benzenoids that prevented us from using the same trick in the benzenoid case. In figure 4 is shown a situation where deletion of the middle edge in a normal block consisting of a hexagon dimer results in a graph that does not satisfy the conditions of Theorem C, since it has an internal vertex of degree 2. Hence, the hexagon dimers cannot be dismissed when counting proper normal blocks.

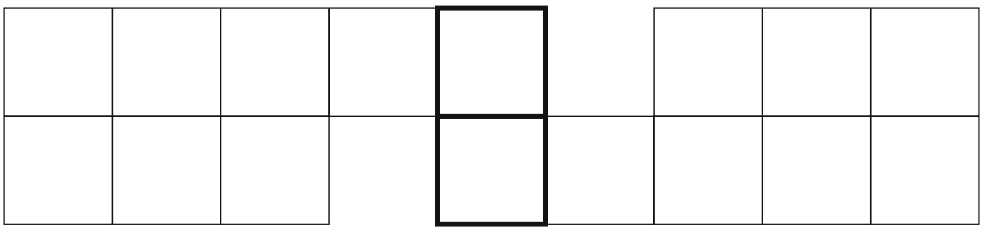

Figure 3. Domino normal block (bold) of a polyomino.

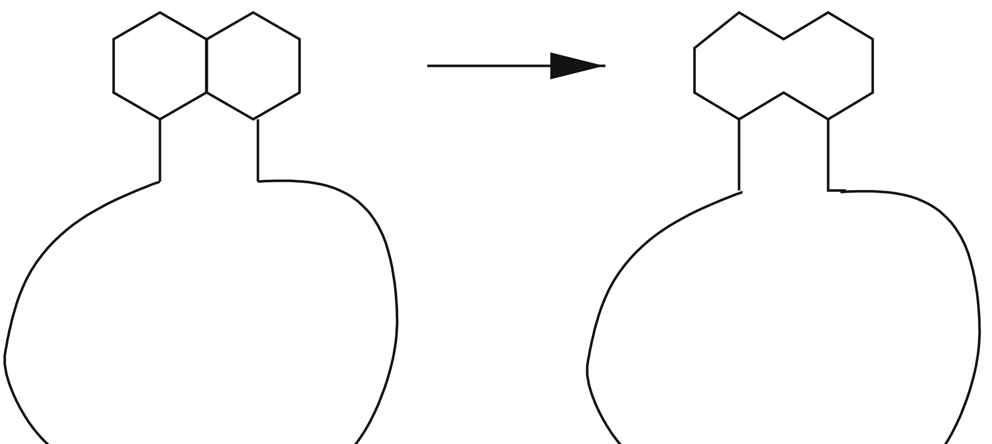

Figure 4. Hexagon dimers are proper normal blocks.

Theorem 4. An essentially disconnected polyomino has at least 16 different perfect matchings.

Proof. It follows from Lemma 3 that any essentially disconnected polyomino must have at least two proper normal blocks. The smallest proper normal block must have at least three squares. There are two such polyominoes, one of them straight with 5 perfect matchings, the other one L-shaped, with 4 perfect matchings. Hence, in the worst case the original polyomino must contain at least 16 different perfect matchings. □

Corollary 5. Let G be a polyomino with a perfect matching and at least 15 squares. Then G has at least 16 perfect matchings. □

As in the benzenoid case, the lower bound of Theorem 4 is the best possible, since for all $n \geqslant 9$ there is a Kekuléan polyomino with n squares and exactly 16 perfect matchings. The first few members of this series of polyominoes are shown in figure 5. The normal blocks are shown in bold.

Again, the list of all polyominoes with less than 16 perfect matchings is finite.

4. Infinite realizability

Motivated by examples from figures 2 and 5, we may ask the following question: For which positive integers n there are infinitely many benzenoids with n perfect matchings? Obviously, the set of such numbers is non-empty, since it contains number nine. Let us call such numbers **infinitely realizable by benzenoids**. The set of positive integers infinitely realizable by polyominoes is defined in an analogous manner. Again, this set is non-empty, since it contains at least the number 16.

It is clear from Theorem A that normal lattice animals cannot contribute to infinite realizability. Hence, no positive integer $n < 9$ is infinitely realizable by benzenoids, and no positive integer $n < 16$ is infinitely realizable by polyominoes. Further, the numbers of perfect matchings in essentially disconnected lattice animals are necessary composite; this follows from Theorem B. Hence, we have established the following result.

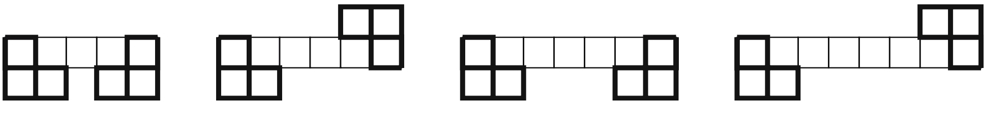

Figure 5. Infinite family of polyominoes with 16 perfect matchings.

Corollary 6. No prime number is infinitely realizable by bipartite lattice animals. □

Corollary 6 solves only a part of our problem. To settle the rest, we treat the benzenoids and the polyominoes separately.

Theorem 7. A positive integer $n \geqslant 9$ is infinitely realizable by benzenoids if and only if it is not of the form $k \cdot p$, where p is a prime number, and $k \in \{1, 2\}$.

Proof. Let $n \in \mathbb{N}$ be of the form $2p$, where p is a prime number. If n is infinitely realizable by benzenoids, then there must be infinitely many essentially disconnected benzenoids with $2p$ perfect matchings. Since p perfect matchings must all be contained in one normal block, the remaining normal block must contain only two perfect matchings. The only normal benzenoid with two perfect matchings is a single hexagon, and this contradicts Theorem C. Together with Corollary 6, this proves that no integer of the form p or $2p$ is infinitely realizable by benzenoids for a prime number p. The claim of the theorem will follow if we show that all other positive integers are infinitely realizable. So, take a positive integer n which is composite and not of the form $2p$ for some prime number p. If n is odd, then it must be of the form $n = pq$, for some odd positive integers p and q. We construct an infinite family of benzenoids with n perfect matchings by connecting two straight linear chains of hexagons of length $p - 1$ and $q - 1$, respectively, by a straight linear chain of hexagons of arbitrary length in the manner shown in figure 6(a). If n is even, then n is of the form $n = 2^p q$, where $p \geqslant 2$ and q is odd. An infinite family of benzenoids with n perfect matchings is constructed in the manner shown in figure 6(b). □

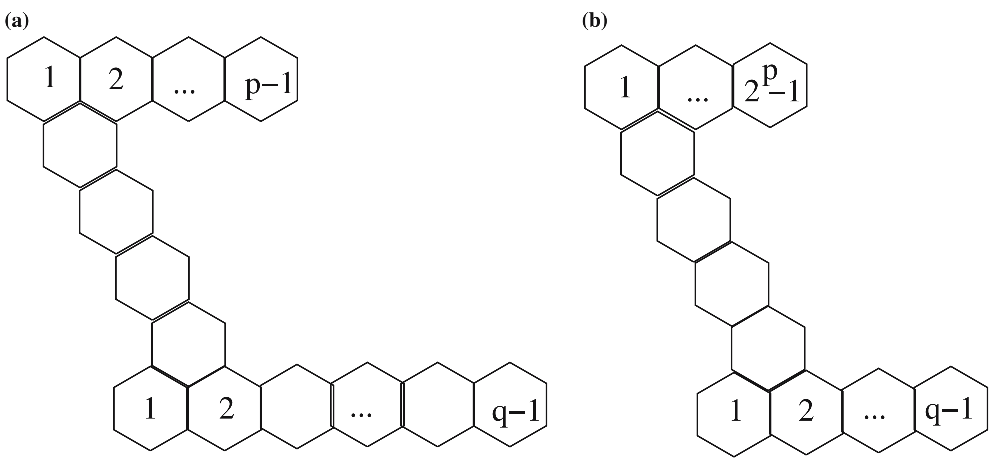

Figure 6. Infinite realizability by benzenoids.

The polyomino case is a bit more complicated, but the proof follows along the same lines.

Theorem 8. A positive integer $n \geqslant 16$, $n \neq 18$, $n \neq 27$, is infinitely realizable by polyominoes if and only if it is not of the form $k \cdot p$, where p is a prime number, and $k \in \{1, 2, 3\}$.

Proof. The impossibility of infinite realizability for the numbers of the form p, $2p$, and $3p$, where p is prime, and for the exceptional cases $n = 18$ and $n = 27$, follows from Theorem C by the same arguments as in the benzenoid case. For any other n we construct an infinite family of polyominoes with n perfect matchings by replacing the normal blocks of polyominoes from figure 5 by zig-zag polyominoes from figure 1 of the appropriate length. □

We conclude this section with a short remark concerning the number one. This is the only positive integer that is not realizable, neither finitely nor infinitely, by bipartite lattice animals. This remark also serves as a bridge toward the next section, where we consider the realizability of zero.

5. Concealed non-Kekuléan polyominoes

Obviously, zero is infinitely realizable by both types of bipartite lattice animals, since there are infinitely many non-Kekuléan benzenoids and polyominoes. The simplest are those constructed by appending a straight linear chain of basic polygons to the basic non-Kekuléan configuration, as shown in figure 7. (The basic non-Kekuléan configurations are shown in bold). This infinite realizability appears, however, rather trivial, since it is obvious that these lattice animals have an odd number of vertices, and hence cannot contain a perfect matching. A bit less trivial are the families shown in figure 8; their members have an even number of vertices, but the classes of bipartition are not of equal size. Again, the basic semi-trivial shapes are shown in bold.

The existence of non-Kekuléan benzenoids with the bipartition classes of equal size (called **concealed** non-Kekuléan benzenoids) has been a part of benzenoid folklore for many decades. The smallest example is shown in figure 9, and an infinite family of such graphs can be constructed by cutting the graph along

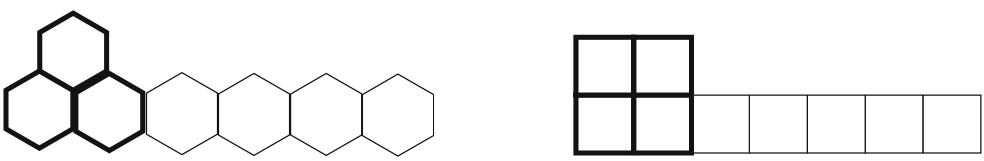

Figure 7. Trivially non-Kekuléan lattice animals.

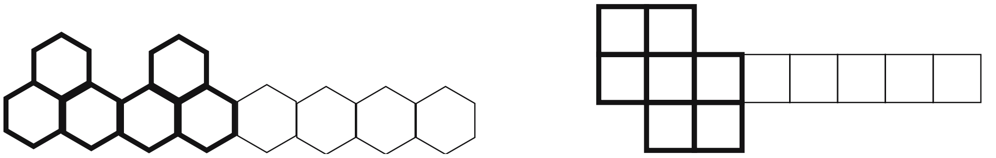

Figure 8. Semi-trivially non-Kekuléan lattice animals.

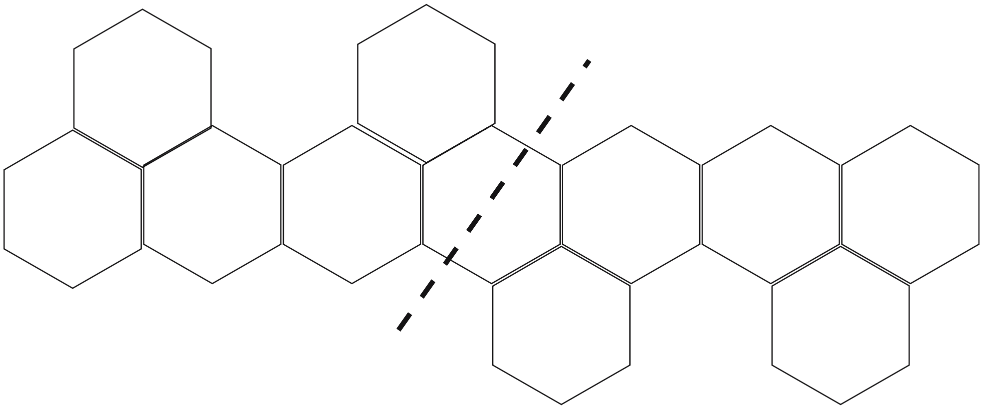

Figure 9. The smallest concealed non-Kekuléan benzenoid.

the dashed line (shown in bold) and inserting a straight linear chain of hexagons of arbitrary length. Hence, zero is non-trivially infinitely realizable by benzenoids. The polyomino case is settled by the following result.

Theorem 9. For each $h \geqslant 15$ there is a concealed non-Kekuléan polyomino on h squares.

Proof. It can be easily checked that the leftmost polyomino in figure 10 is concealed non-Kekuléan. Both properties are retained by all members of the family constructed by lengthening the “bridge” between two copies of the basic semi-trivial shape and reflecting one of them for even lengths of the bridge. □

Corollary 10. Zero is non-trivially infinitely realizable by bipartite lattice animals. □

The leftmost polyomino in figure 10 is the smallest possible, in the sense that no concealed non-Kekuléan polyomino can have less than 15 squares.

Theorem 11. The smallest possible concealed non-Kekuléan polyomino has 15 squares.

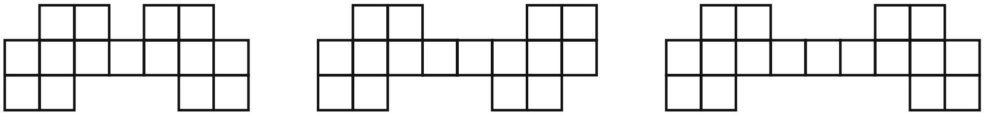

Figure 10. Infinite family of concealed non-Kekuléan polyominoes.

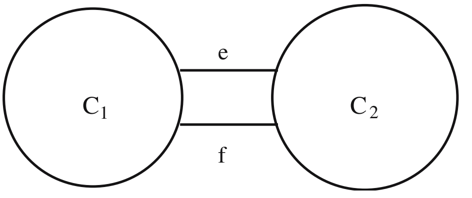

Figure 11. The structure of the smallest concealed non-Kekuléan polyomino.

Proof. An **edge cut** in a graph G is a set C of edges whose removal disconnects G. (We remove only the edges, their end-vertices are not removed). We start by showing that a minimal (in the sense of the number of squares) concealed non-Kekuléan polyomino must have an edge cut that consists of two parallel edges of a single square. Let us suppose that such an edge cut does not exist in a minimal concealed non-Kekuléan polyomino P. Let us orient P in the plane so that its edges run vertically and horizontally. Then P must have either a vertical or a horizontal edge cut that has more than two edges. Let C be any such cut. At least two edges of C lye on the outer boundary of P. Removal of one of these two edges will affect neither the concealedness nor the non-Kekulénicity of P, and will result in a polyomino with the same properties that has one square less than P, contradicting the assumption of minimality. Hence, any minimal concealed non-Kekuléan polyomino must be of the form shown in figure 11.

Next we show that for each of the components C_1 and C_2 the classes of respective bipartitions must differ in size by at least two. As the total number of vertices must be even, the numbers of vertices in C_1 and C_2 must be of the same parity. Let us suppose that they are odd. Then the surplus of black vertices in C_1 must be exactly balanced by the surplus of white vertices in C_2. Let this surplus be equal to one. Consider the black vertex in C_1 that is connected to a white vertex in C_2 by the edge e from the edge cut $C = \{e, f\}$. By removing the edge e together with its endpoints and the edge f without its endpoints, we obtain two polyominoes, C_1' and C_2'. If both of them have a perfect matching, then the union of these matchings together with the edge e would make a perfect matching in P, a contradiction with the non-Kekulénicity of P. Hence, at least one of C_1' and C_2' must be non-Kekuléan. Let it be C_1'. But then, the number of vertices of C_1' is even, and the classes of bipartition are of equal size, and this makes C_1' a concealed non-Kekuléan polyomino strictly smaller than P, again a contradiction. Hence, both C_1 and C_2 must have an even number of vertices. If we suppose that the classes of bipartition of, say, C_1 are of equal size, then the same must be valid for C_2. Since P was non-Kekuléan, at least one of C_1 and C_2 must be non-Kekuléan, thus contradicting the minimality of P. Hence, the classes of bipartition in C_1 and C_2 must be even and differ in size by at least two. The smallest such polyomino has at least 7 squares, and the claim of the theorem follows. □

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