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**LINEAR ALGORITHM FOR
ZHANG-ZHANG
POLYNOMIAL OF
CATACONDENSED
HEXAGONAL SYSTEMS**

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Linear algorithm for Zhang-Zhang polynomial of catacondensed hexagonal systems

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Abstract

The Zhang-Zhang polynomial is a relatively new polynomial related to hexagonal systems. It is based on the Kekulé and Clar structures of the underlying benzenoid molecule. We present an optimal algorithm to compute the Zhang-Zhang polynomial in a catacondensed hexagonal system. The algorithm can be used to simultaneously compute several important invariants such as the Clar number, the number of Kekulé structures and the first Herndon number of a catacondensed hexagonal system in linear time.

Key words: Zhang-Zhang polynomial, catacondensed hexagonal system, algorithm

1 Introduction

A *hexagonal system* or a *benzenoid system* is a finite connected plane graph with no cut vertices in which every interior region is bounded by a regular hexagon of a side length one. Hexagonal system can be constructed as follows. Let Z be a circuit on the benzenoid (graphite) lattice. Then a hexagonal system is formed by the vertices and edges of the lattice lying on Z and in the interior of Z . A subgraph of a hexagonal system is called a *generalized hexagonal system*. A hexagonal system H is *catacondensed* if any triple of hexagons of H has empty intersection (see Fig. 1).

It is well known that hexagonal systems possess very natural chemical background. In particular, the carbon-atom skeleton of a benzenoid hydrocarbon is a hexagonal system

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[3, 5]. Therefore hexagonal systems and their mathematical properties were much studied in chemistry.

The Chinese mathematicians Heping Zhang and Fuji Zhang conceived a combinatorial polynomial associated with hexagonal systems and underlying benzenoid molecules. The authors provided some fundamental results and also reported some chemical applications of their polynomial [10, 11], while intensive research along these lines started quite recently [1, 6, 7, 8].

The polynomial put forward by Zhang and Zhang will be referred to as the Zhang-Zhang polynomial, and will be denoted by $\zeta(H, x)$ for a hexagonal system H .

The paper is organized as follows. In the next section we first give definitions and concepts needed in this paper. We then present the main theorem: the recurrence relation in which the induced subgraphs are again catacondensed hexagonal systems of smaller size. The theorem is illustrated with two examples, while its proof is given in Section 3. Using this result, we present in Section 4 an optimal (a linear) algorithm for computing the Zhang-Zhang polynomial of a catacondensed hexagonal system.

2 Preliminaries and the main result

A *matching* of a graph G is a set of pairwise independent edges. A matching is a *1-factor*, if it covers all the vertices of G .

In chemistry instead of 1-factors one speaks of Kekulé structures and the edges contained in a perfect matching are referred to as the double bonds of the respective Kekulé structure. A hexagonal system which admits at least one Kekulé structure is called *Kekuléan*.

The Zhang-Zhang polynomial is defined in the following manner. Let H be a Kekuléan hexagonal system. A *Clar cover* C of H is a spanning subgraph of H , each component of which is either a hexagon or an edge. Let $h(C)$ denote the number of hexagons of C . Set $\sigma(H) = \max \{h(C) : C \text{ is a Clar cover of } H\}$, which is called the *Clar number* of H . Let $z(H, i)$ be the number of Clar covers of H , containing exactly i hexagons. Then

$$\zeta(H, w) = \sum_{i=0}^{\sigma(H)} \sigma(H, i) w^i.$$

This Zhang-Zhang polynomial contains information on the number of Kekulé structures, the Clar number, the number of Clar formulas and the Hosoya-Yamaguchi sextet polynomial $\sigma(H, w)$ [5], and several other important characteristics of the underlying benzenoid molecule.

A hexagon which shares an edge with exactly one other hexagon is called *pendant*.

Let h denote a hexagon of a generalized hexagonal system H . Then $H - h$ denote a subgraph of H obtained by deleting all the vertices of h together with their incident edges.

The following three results presented in [10] provide the foundation for the main result.

Theorem 1. *Let H be a generalized hexagonal system, the components of which are H_1, H_2, \dots, H_s . Then $\zeta(H, w) = \prod_{i=1}^s \zeta(H_i, w)$.*

Theorem 2. *Let H be a generalized hexagonal system. Assuming that xy is an edge of a hexagon s of H which lies on the periphery of H , then $\zeta(H, w) = w\zeta(H - s, w) + \zeta(H - x - y, w) + \zeta(H - xy, w)$.*

Theorem 3. *Let H be a generalized hexagonal system and xy be an edge not belonging to any hexagon of H . Then $\zeta(H, w) = \zeta(H - x - y, w) + \zeta(H - xy, w)$.*

We now recall some notations concerning catacondensed hexagonal systems introduced in [9].

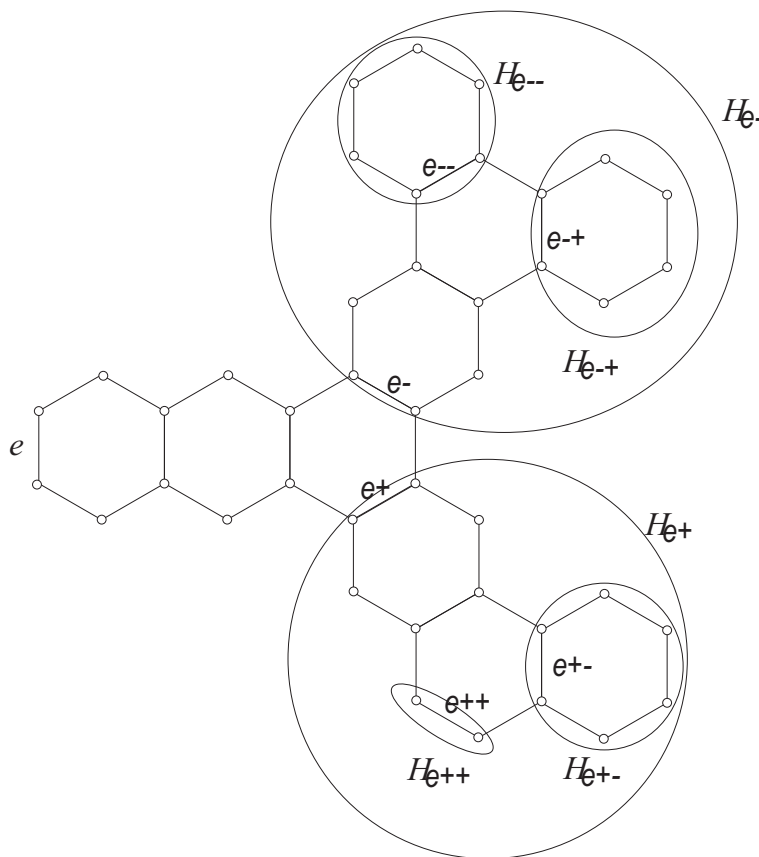


Figure 1: Catacondensed hexagonal system H .

Let e be an edge of a hexagonal system H . Then the *cut* C_e corresponding to e is the set of edges so that with every edge e' of C_e also the opposite edge with respect to a hexagon containing e' belongs to C_e .

Let H be a catacondensed hexagonal system and e an edge of H with ends of degree two. Let $e = e_0, e_1, \dots, e_n$ be the edges of the cut C_e , and let $h_1 = h, h_2, \dots, h_n$ be the corresponding hexagons. Let $e+$ and $e-$ be the edges of h_n adjacent to e_n , where $e+$ is the right edge looking from $e = e_0$ to e_n while $e-$ is the left edge, and let h_+ and h_- be the corresponding hexagons. Remove now from G the hexagons h_1, \dots, h_n , except $e+$ and $e-$. Then the remaining graph consists of two connected components H_{e+} and H_{e-} , where $e+ \in H_{e+}$ and $e- \in H_{e-}$. Note that any of H_{e+} and H_{e-} is either a hexagonal system or a K_2 . These notations are illustrated in Fig. 1. If H_{e+} is a catacondensed hexagonal system, we repeat the described construction on H_{e+} , where the construction begins with $e+$. In this way we obtain two connected subgraph of H denoted H_{e++} and H_{e+-} . Similarly, if H_{e-} is a catacondensed hexagonal system, then we repeat the construction on H_{e-} , starting with $e-$, to obtain connected subgraphs H_{e-+} and H_{e--} . In the case that $H_{e+} = K_2$ we set $H_{e++} = K_2$ and $H_{e+-} = K_2$, and if $H_{e-} = K_2$ we set $H_{e-+} = K_2$ and $H_{e--} = K_2$.

Now we are ready to state:

Theorem 4. *Let H be a catacondensed hexagonal system and e the edge with ends of degree two with $|C_e| = n + 1$, where $n \geq 1$. Then*

$$\zeta(H, w) = (nw - w + n)\zeta(H_{e+}, w)\zeta(H_{e-}, w) + (w + 1)\zeta(H_{e++}, w)\zeta(H_{e+-}, w)\zeta(H_{e-+}, w)\zeta(H_{e--}, w).$$

Theorem 4 is proved in the next section, in the rest of this section we illustrate it with two examples.

A *hexagonal chain* is a catacondensed hexagonal system such that it has no hexagon with more than two adjacent hexagons. Let a hexagon h of a catacondensed hexagonal system be adjacent to exactly two other hexagons. Then h possesses two vertices of degree 2. If these two vertices are adjacent, h is called *angularly connected*, otherwise it is *linearly connected*. A hexagonal chain is *linear* if every hexagon, apart from a pendant one, is linearly connected. A linear hexagonal chain on n hexagons is denoted L_n .

Example 1 Let e be an edge of L_n that induces $|C_e| = n + 1$. Then from Theorem 4 easily follows that

$$\zeta(L_n, w) = nw - w + n + w + 1 = n + 1 + nw.$$

Example 2 Consider the graph H from Fig. 1. For the edge e of H we get

$$\zeta(H, w) = (2w + 3)\zeta(H_{e+}, w)\zeta(H_{e-}, w) + (w + 1)\zeta(H_{e++}, w)\zeta(H_{e+-}, w)\zeta(H_{e-+}, w)\zeta(H_{e--}, w)$$

where

$$\begin{aligned}\zeta(H_{e_{++}}, w) &= 1, & \zeta(H_{e_{+-}}, w) &= \zeta(L_1, w) = 2 + w, \\ \zeta(H_{e_{-+}}, w) &= \zeta(L_1, w) = 2 + w, & \zeta(H_{e_{--}}, w) &= \zeta(L_1, w) = 2 + w.\end{aligned}$$

We then get

$$\zeta(H_{e_+}, w) = (w + 2)(w + 2)(w + 2) + (w + 1) = 9 + 13w + 6w^2 + w^3 \text{ and}$$

$$\zeta(H_{e_-}, w) = (w + 2)(w + 2) + (w + 1) = 5 + 5w + w^2.$$

Thus we have

$$\zeta(H, w) = 143 + 440w + 550w^2 + 359w^3 + 130w^4 + 25w^5 + 2w^6.$$

3 Proof of the main result

In order to obtain the proof of the theorem we need the definitions and two lemmas presented below.

The edge of a pendant hexagon that is shared with another hexagon will be called a *join edge*.

Let h' denote a pendant hexagon of H . Then $H \setminus h'$ denote a subgraph of H obtained by deleting the vertices of h' with the exception of the vertices of the join edge.

Let H' denote a subgraph of a generalized hexagonal system H and let uv be an edge of H , such that $v \in V(H')$ and $u \in V(H) \setminus V(H')$. Then $H' + uv$ denote a graph with the vertex set $V(H') \cup \{u\}$ and the set of edges $E(H') \cup \{uv\}$.

Lemma 1. *Let H be a catacondensed hexagonal system and $e = xy$ the edge with ends of degree two with $|C_e| = n + 1$, where $n \geq 1$. Then $\zeta(H - x - y, w) = \zeta(H_{e_+}, w)\zeta(H_{e_-}, w)$.*

Proof. Let $e = e_0, e_1, \dots, e_n$ be edges of C_e with $e_i = x_i y_i$, $1 \leq i \leq n$, and h_1, h_2, \dots, h_n be hexagons induced by C_e . We then define $G_1 = H - x - y$, while for $i > 1$ the graph G_i is obtained from H by removing all vertices of hexagons $h_1, h_2 \dots h_{i-1}$.

Suppose first that $n = 1$. From Theorem 3 it follows that $\zeta(G_1, w) = \zeta(G_1 - x_1 - y_1, w) + \zeta(G_1 - x_1 y_1, w)$. Note that $G_1 - x_1 - y_1$ possesses two connected component, say $H_{e_+} - x_1$ and $H_{e_-} - y_1$. Since H_{e_+} (resp. H_{e_-}) is a catacondensed hexagonal systems and therefore it admits a 1-factor, $H_{e_+} - x_1$ (resp. $H_{e_-} - y_1$) cannot induce a 1-factor. It follows that $\zeta(G_1 - x_1 - y_1, w) = 0$ and $\zeta(G_1, w) = \zeta(G_1 - x_1 y_1, w)$. The connected components of $G_1 - x_1 y_1$ are H_{e_+} and H_{e_-} . From Theorem now it follows that $\zeta(G_1, w) = \zeta(H_{e_+}, w)\zeta(H_{e_-}, w)$ and this case is settled.

Let $n > 1$ and let x', y' denote the vertices of degree one in G_1 . Let also x' and y' be adjacent to x_1 and y_1 , respectively. Then from Theorem 3 it follows that $\zeta(G_1, w) =$

$\zeta(G_1 - x' - x_1, w) + \zeta(G_1 - x'x_1, w)$. Note that $G_1 - x'x_1$ does not admit a 1-factor, therefore $\zeta(G_1, w) = \zeta(G_1 - x' - x, w)$. Analogously, $G_1 - x' - x_1 - y'y_1$ does not admit a 1-factor and we get $\zeta(G_1 - x' - x_1, w) = \zeta(G_1 - x' - x_1 - y' - y_1, w) + \zeta(G_1 - x' - x_1 - y'y_1, w) = \zeta(G_1 - x' - x_1 - y' - y_1, w)$. Note that $G - x' - x_1 - y' - y_1 = G_2$ is again a graph with two vertices of degree one. Moreover, if $n = 2$, then analogously as for the case $n = 1$ we get $\zeta(G_1, w) = \zeta(G_2, w) = \zeta(H_{e+}, w)\zeta(H_{e-}, w)$. If $n > 2$, we repeat the above procedure to obtain $\zeta(G_1, w) = \zeta(G_2, w) = \dots = \zeta(G_{n-1}, w) = \zeta(H_{e+}, w)\zeta(H_{e-}, w)$ and the assertion follows. \square

Lemma 2. *Let H be a catacondensed hexagonal system and $e = xy$ be the edge with ends of degree two with $|C_e| = n + 1$, where $n \geq 1$. Then*

$$\zeta(H - xy, w) = \begin{cases} \zeta(H \setminus h_1, w) & \text{if } n > 1 \\ \zeta(H_{e++}, w)\zeta(H_{e+-}, w)\zeta(H_{e-+}, w)\zeta(H_{e--}, w) & \text{if } n = 1 \end{cases}$$

Proof. Let x' (resp. y') denote the vertex of $H - xy$ adjacent to x (resp. y).

Let $n > 1$. From Theorem 3 it follows that $\zeta(H - xy, w) = \zeta(H - xy - x - x', w) + \zeta(H - xy - xx', w) = \zeta(H - xy - x - x', w) = \zeta(H - x - x', w)$. Analogously, $\zeta(H - x - x', w) = \zeta(H - x - x' - y - y', w) + \zeta(H - x - x - yy', w) = \zeta(H - x - x' - y - y', w)$. Since $H - x - x' - y - y' = H \setminus h_1$, this case is settled.

Let $n = 1$ and let x_1, y_1 denote the endvertices of e_1 . Then from Theorem 3 it follows that $\zeta(H - xy, w) = \zeta(H - xy - x_1 - y_1, w) + \zeta(H - xy - x_1y_1, w)$. The graph $H - xy - x_1y_1$ has two connected components: $H_{e+} + xx'$ and $H_{e-} + yy'$. Since H_{e+} (resp. H_{e-}) is either a catacondensed hexagonal system or K_2 and therefore it admits a 1-factor, $H_{e+} + xx'$ (resp. $H_{e-} + yy'$) cannot induce a 1-factor. It follows that $\zeta(H - xy, w) = \zeta(H - xy - x_1 - y_1, w)$. The graph $H - xy - x_1 - y_1$ possesses two connected components, say H'_{e+} and H'_{e-} , where $H'_{e+} = H_{e+} + xx' - x_1$ and $H'_{e-} = H_{e-} + yy' - y_1$. From Theorem 3 then it follows that

$$\zeta(H - xy, w) = \zeta(H - xy - x_1 - y_1, w) = \zeta(H'_{e+}, w)\zeta(H'_{e-}, w). \quad (1)$$

We first compute $\zeta(H'_{e+}, w)$.

If $H_{e+} = K_2$, then $H'_{e+} = K_2$ and we get $\zeta(H'_{e+}, w) = 1$. Since for $H_{e+} = K_2$ we defined $H_{e++} = H_{e+-} = K_2$, we can write $\zeta(H'_{e+}, w) = \zeta(H_{e++}, w)\zeta(H_{e+-}, w)$.

If H_{e+} is a catacondensed hexagonal system, then Theorem 3 yields $\zeta(H'_{e+}, w) = \zeta(H'_{e+} - x - x', w) + \zeta(H'_{e+} - xx', w) = \zeta(H'_{e+} - x - x', w) = \zeta(H_{e+} - x' - x_1, w)$. From Lemma 1 then it follows $\zeta(H_{e+} - x' - x_1) = \zeta(H_{e++}, w)\zeta(H_{e+-}, w)$.

Analogously we get $\zeta(H'_{e-}, w) = \zeta(H_{e-+}, w)\zeta(H_{e--}, w)$ and the assertion now follows from Equation 1. \square

We are ready now to prove Theorem 4.

Proof. Let $e = e_0, e_1, \dots, e_{n+1}$ be the edges of C_e and h_1, h_2, \dots, h_n be hexagons induced by C_e . Let also $e = xy$ and let x' (resp. y') denote the vertex of $H - xy$ adjacent to x (resp. y).

From Theorem 2 it follows

$$\zeta(H, w) = w\zeta(H - h_1, w) + \zeta(H - x - y, w) + \zeta(H - xy, w). \quad (2)$$

Moreover, Lemma 1 yields $\zeta(H - x - y, w) = \zeta(H_{e+}, w)\zeta(H_{e-}, w)$.

The rest of the proof is by induction on n .

Suppose first that $n = 1$. Let $e+ = x'x_1$ and $e- = y'y_1$. Then from Lemma 2 it follows that $\zeta(H - xy, w) = \zeta(H_{e++}, w)\zeta(H_{e+-}, w)\zeta(H_{e-+}, w)\zeta(H_{e--})$. Since the graph $H - h_1$ possesses two connected components, say H_{e+}^- and H_{e-}^- , where $H_{e+}^- = H_{e+} - x' - x_1$ and $H_{e-}^- = H_{e-} - y' - y_1$, from Lemma 1 and Theorem 3 it follows that $\zeta(H - h_1, w) = \zeta(H_{e+} - x' - x_1)\zeta(H_{e-} - y' - y_1) = \zeta(H_{e++}, w)\zeta(H_{e+-}, w)\zeta(H_{e-+}, w)\zeta(H_{e--})$. We then get from Equation 2

$$\zeta(H, w) = \zeta(H_{e+}, w)\zeta(H_{e-}, w) + (w + 1)\zeta(H_{e++}, w)\zeta(H_{e+-}, w)\zeta(H_{e-+}, w)\zeta(H_{e--})$$

and this case is settled.

Let $n > 1$. Suppose also that the theorem holds for $n - 1$. Note first that $\zeta(H - xy, w) = \zeta(H \setminus h_1, w)$ by Lemma 2. Note also that $H - h_1 = (H \setminus h_1) - x_1 - y_1$. Since $H \setminus h_1$ is a catacondensed hexagonal system and x_1y_1 its edge with ends of degree two, from Lemma 1 it follows that $\zeta(H - h_1) = \zeta(H_{e+}, w)\zeta(H_{e-}, w)$.

By combining the results from above in Equation 2 we now get

$$\zeta(H, w) = w(\zeta(H_{e+}, w)\zeta(H_{e-}, w)) + \zeta(H_{e+}, w)\zeta(H_{e-}, w) + \zeta(H \setminus h_1, w).$$

Moreover, the induction hypothesis yields

$$\begin{aligned} \zeta(H \setminus h_1, w) &= (nw - 2w + n - 1)\zeta(H_{e+}, w)\zeta(H_{e-}, w) \\ &\quad + (w + 1)\zeta(H_{e++}, w)\zeta(H_{e+-}, w)\zeta(H_{e-+}, w)\zeta(H_{e--}, w) \end{aligned}$$

and the assertion easily follows. \square

4 Algorithm

Theorem 2 gives the recurrence relation by which the Zhang-Zhang polynomial of a hexagonal system H can be computed. An associated recursive technique is described in [6].

However, a straightforward application of Theorem 2 is problematic from the algorithmic point of view since the three subgraphs generated by applying the theorem are not hexagonal systems (they are generalized hexagonal systems). Moreover, the obtained subgraphs are nearly of the same size (in the number of vertices and edges) and not much smaller than H . It follows that a straightforward algorithm cannot be efficient. Furthermore, one can expect that such an algorithm run in superpolynomial time (e.g. [2, Section 16.2]) for a general hexagonal system.

We will show that Theorem 4 can lead to a dynamic algorithm, which computes the Zhang-Zhang polynomial of a catacondensed hexagonal system in linear (optimal) time. The reason for the effectiveness of an algorithm is the fact that the subgraphs generated by the theorem are again catacondensed hexagonal systems but of smaller size. In this context, a dynamic algorithm computes Zhang-Zhang polynomial of every subgraph only once, thereby avoiding the work of recomputing for nearly identical subgraphs.

Procedure ZHANG;

Input: catacondensed hexagonal system H ; an edge with ends of degree two e

Output: $\zeta(H, w)$, $\zeta(H_{e+}, w)$, $\zeta(H_{e-}, w)$;

begin

1. **if** $H = K_2$ **then begin**

$\zeta(H, w) := 1$; $\zeta(H_{e+}, w) := 1$; $\zeta(H_{e-}, w) := 1$; **exit**(ZHANG); **end**;

2. Determine: H_{e+} , H_{e-} , and $|C_e| = n + 1$;

3. ZHANG(H_{e+} , $e+$, $\zeta(H_{e+}, w)$, $\zeta(H_{e++}, w)$, $\zeta(H_{e+-}, w)$);

4. ZHANG(H_{e-} , $e-$, $\zeta(H_{e-}, w)$, $\zeta(H_{e-+}, w)$, $\zeta(H_{e--}, w)$);

5. $\zeta(H, w) := (nw - w + n)\zeta(H_{e+}, w)\zeta(H_{e-}, w)$
 $+ (w + 1)\zeta(H_{e++}, w)\zeta(H_{e+-}, w)\zeta(H_{e-+}, w)\zeta(H_{e--}, w)$;

end.

Theorem 5. *Let H be a catacondensed hexagonal system. Then ZHANG finds the Zhang-Zhang polynomial of H in linear time.*

Proof. The algorithm in Step 1 checks if $H = K_2$. If this is the case, then $\zeta(H, w)$, $\zeta(H_{e+}, w)$ and $\zeta(H_{e-}, w)$ get the value 1 and we exit the procedure. The correctness of this step follows from the definition of graphs H_{e+} and H_{e-} .

If H is a catacondensed hexagonal system, the procedure recursively finds $\zeta(H_{e+}, w)$, $\zeta(H_{e-}, w)$, $\zeta(H_{e++}, w)$, $\zeta(H_{e+-}, w)$, $\zeta(H_{e-+}, w)$ and $\zeta(H_{e--}, w)$. This values are used in the Step 5 of the algorithm the correctness of which follows from Theorem 4.

In order to prove the complexity of the algorithm, note first that the number of hexagons of H is linear in the number of vertices of H . In order to compute H_{e+} and H_{e-} the procedure computes the hexagons induced by the cut C_e . Note that for a given edge

e of H , the opposite edge with respect to a hexagon containing e can clearly be found in constant time. The edges of C_e and the corresponding hexagons can be therefore found in time which is linear in the number of edges of C_e . We can also see that each hexagon of H is involved in exactly one such computation. Therefore, we may assume that the overall complexity of the procedure is linear and the proof is completed. \square

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