Anti–Forcing Number of Some Specific Graphs

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ARTICLE INFO

Article History:
Received 9 September 2016
Accepted 14 March 2017
Published online 31 August 2017

Keywords:
Anti–forcing number
Anti–forcing set
Corona product

ABSTRACT

Let \( G \) be a simple connected graph. A perfect matching (or Kekulé structure in chemical language) of \( G \) is a set of disjoint edges which covers all vertices of \( G \). The anti–forcing number of \( G \) is the smallest number of edges such that the remaining graph obtained by deleting these edges has a unique perfect matching and is denoted by \( af(G) \). In this paper we consider some specific graphs that are of importance in chemistry and study their anti–forcing numbers.

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1. INTRODUCTION

All graphs considered in this paper are undirected and simple. Let \( G \) be a simple graph with vertex set \( V(G) \) and edge set \( E(G) \). A perfect matching or 1–factor (or Kekulé structure in chemical literature) of \( G \) is a set of disjoint edges which covers all vertices of \( G \). Perfect matching has many practical applications, such as in dimer problem of statistical physics, Kekulé structures in organic chemistry and personnel assignment of operations research, etc. For more details on perfect matching, we refer the reader to see [8].

In 2007, Vukičević and Trinajstić [9,10] introduced the anti–forcing number of a graph \( G \) with perfect matching \( M \). A set \( S \subseteq M \) is called a forcing set of \( M \) if \( S \) cannot be contained in another perfect matching of \( G \) other than \( M \). The forcing number (or innate degree of freedom) of \( M \) is defined as the minimum size of all forcing sets of \( M \), denoted by \( f(G,M) \) [5, 6]. The minimum forcing number of \( G \) is the minimum value of the

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DOI: 10.22052/ijmc.2017.60978.1235
forcing numbers of all perfect matchings of $G$, denoted by $f(G)$. Zhang et al. [11] proved that the minimum forcing number of fullerenes has a lower bound three and there are infinitely many fullerenes achieving this bound. For $S \subseteq E(G)$, let $G - S$ denote the graph obtained by removing $S$ from $G$. Then $S$ is called an anti–forcing set if $G - S$ has a unique perfect matching. The cardinality of a smallest anti–forcing set is called the anti–forcing number of $G$, denoted by $af(G)$. An edge $e$ of $G$ is called an anti–forcing edge if $G - e$ has a unique perfect matching. Note that $af(G) = |E(G)|$ if and only if $G$ does not have any perfect matching. A graph $G$ is called odd or even graph, if the number of vertices of $G$ is odd or even, respectively.

Recently, Lei et al. [7] defined the anti–forcing number of a perfect matching $M$ of a graph $G$ as the minimal number of edges not in $M$ whose removal to make $M$ as a single perfect matching of the resulting graph, denoted by $af(G, M)$. By this definition, the anti–forcing number of a graph $G$ is the smallest anti–forcing number over all perfect matchings of $G$.

In the next section, after computing the anti–forcing number of some specific graphs, the anti–forcing number of the link and the chain of graphs are discussed. Also we study the anti–forcing number of chain triangular cactus and chain square cactus as a special kind of the chain of graphs that are of importance in chemistry. In Section 3, we consider two graph operations, the join and the corona of two graphs and obtain some relations between the anti–forcing number of two graphs $G_1$ and $G_2$ and the anti–forcing number of the join and the corona of them under some suitable assumptions. Finally, in Section 4, we compute the anti–forcing number of some dendrimers.

2. Anti–Forcing Number of Specific Graphs

In this section, we shall compute the anti–forcing number of some specific graphs. First we consider some certain graphs such as paths, cycles, wheels, friendship and Dutch–windmill graphs. The following example gives the anti–forcing number of path, cycle and wheel graphs.

**Example 2.1** Let $P_n$, $C_n$ and $W_n$ be a path, cycle and wheel of order $n$, respectively. We have

$$af(P_n) = \begin{cases} n - 1 & 2 \nmid n, \\ 0 & 2 \nmid n \end{cases}, af(C_n) = \begin{cases} n & 2 \nmid n, \\ 1 & 2 \nmid n \end{cases} \text{ and } af(W_n) = \begin{cases} 2(n - 1) & 2 \nmid n, \\ 2 & 2 \nmid n \end{cases}.$$  

As another specific graph, we consider friendship graph $F_n$ which is a graph that can be constructed by coalescence $n$ copies of the cycle graph $C_3$ with a common vertex. It is obvious that this graph does not have any perfect matching and so
For the stars graphs $K_{1,n}$ there is no perfect matching, thus $af(S_n) = n$, for $n \geq 2$ and $af(K_{1,1}) = 0$. Also for the $n$–book graph $B_n$ which can be constructed by joining $n$ copies of the cycle graph $C_4$ with a common edge $\{u,v\}$, $af(B_n) = 1$.

Let $Wd(k,n)$ be an undirected graph, constructed for $k \geq 2$ and $n \geq 2$ by joining $n$ copies of the complete graph $K_k$ at a shared vertex. We have $|V(G)| = (k-1)n + 1$, $|E(G)| = 1/2kn(k-1)$ (see [4]). We have the following theorem for the anti–forcing number of $Wd(k,n)$.

**Theorem 2.2** $af(Wd(k,n)) = \frac{1}{2}kn(k-1)$.

**Proof.** Suppose that $n$ is even. Obviously, for every $k$, $Wd(k,n)$ is an odd graph and so the graph does not have any perfect matching. It implies that for every $k$, $af(Wd(k,n)) = 1/2kn(k-1)$. Now assume that $n$ is odd, then for odd $k$, the order of $Wd(k,n)$ is odd too and hence the graph does not have any perfect matching. For even $k$, using Tutte’s Theorem we have the same result. So we can conclude that $af(Wd(k,n)) = 1/2kn(k-1)$. ■

Here, we consider some graphs with specific construction that are of importance in chemistry and study their anti–forcing number. First we define the link of graphs.

**Definition 2.3** [3] Let $G_1, G_2, ..., G_k$ be a finite sequence of pairwise disjoint connected graphs and let $x_i, y_i \in V(G_i)$. The link $G$ of the graphs $\{G_i\}_{i=1}^k$ with respect to the vertices $\{x_i, y_i\}_{i=1}^k$ is obtained by joining an edge the vertex $y_i$ of $G_i$ with the vertex $x_{i+1}$ of $G_{i+1}$ for all $i = 1, 2, ..., k-1$ (see Figure 1 for $k = 4$).

![Figure 1](image)

**Figure 1:** A link of four graphs.

**Theorem 2.4** Let $L(G_1, G_2, ..., G_k)$ be the link of $k$ graphs $G_1, G_2, ..., G_k$. If every $G_i$ ($1 \leq i \leq k$) has perfect matching, then
\[ af(L(G_1, G_2,\ldots, G_k)) = \sum_{i=1}^{k} af(G_i). \]

**Proof.** It suffices to prove the theorem for \( k = 2 \). Let \( G_1 \) and \( G_2 \) be two graphs with perfect matching. Let \( x_1 \in V(G_1), \ x_2 \in V(G_2) \) and \( L(G_1, G_2) \) be the link of these two graphs obtained by joining an edge the vertex \( x_1 \) with the vertex \( x_2 \). Suppose that \( S_1 \) and \( S_2 \) have the smallest cardinality over all anti–forcing sets of graphs \( G_1 \) and \( G_2 \), respectively. So \( af(G_i) = |S_i| \) and \( af(G_j) = |S_j| \). It is obvious that the edge \( x_1x_2 \) does not belong to any perfect matching of \( L(G_1, G_2) \). So if \( S \) has the smallest cardinality over all anti–forcing sets of graph \( L(G_1, G_2) \), then \( S = S_1 \cup S_2 \) and so,

\[ af(L(G_1, G_2)) = |S| = |S_1| + |S_2| = af(G_1) + af(G_2), \]

which completes our argument. \( \blacksquare \)

Note that if there exist \( 1 \leq i \leq k \) such that \( G_i \) does not have any perfect matching, then Theorem 2.4 is not true. For example, \( af(L(P_3, C_4, C_4)) = 12 \), but \( af(P_3) + 2af(C_4) = 4 \). Now, we consider the chain of graphs and study the anti–forcing number of them for different cases.

**Definition 2.5** [3] Let \( G_1, G_2, \ldots, G_k \) be a finite sequence of pairwise disjoint connected graphs and let \( x_i, y_i \in V(G_i) \). The chain \( G \) of the graphs \( \{G_i\}_{i=1}^{k} \) with respect to the vertices \( \{x_i, y_i\}_{i=1}^{k} \) is obtained by identifying the vertex \( y_i \) with the vertex \( x_{i+1} \) for \( 1 \leq i \leq k-1 \), see Figure 2 for \( k = 4 \).

![Figure 2: A chain of four graphs.](image)

**Theorem 2.6** Let \( C(G_1, G_2,\ldots, G_k) \) be the chain of \( k \) graphs \( G_1, G_2,\ldots, G_k \).

1. If \( G_1, G_2,\ldots, G_k \) are odd graphs, then \( af(C(G_1, G_2,\ldots, G_k)) = \sum_{i=1}^{k} |E(G_i)| \).
2. If \( G_1, G_2,\ldots, G_k \) are even graphs, then for every even \( k \) we have
   \[ af(C(G_1, G_2,\ldots, G_k)) = \sum_{i=1}^{k} |E(G_i)|. \]
Proof.

i. It can easily verified that \(|V(C(G_1,G_2,\ldots,G_k))| = \sum_{i=1}^{k} |V(G_i)|-(k-1)|. Thus in this
case, for every \( k \), \( C(G_1,G_2,\ldots,G_k) \) is an odd graph and so
\[ af(C(G_1,G_2,\ldots,G_k)) = |E(C(G_1,G_2,\ldots,G_k))| \]

Since \(|E(C(G_1,G_2,\ldots,G_k))| = \sum_{i=1}^{k} |E(G_i)|\), we have the result.

ii. It is easy to see that in this case the chain graph \( C(G_1,G_2,\ldots,G_k) \) is an odd graph
and so we have the result.

Hence the result. ■

Remark 2.7 Theorem 2.6(ii), is not true for odd \( k \). For example, \( af(C(P_2,P_4,P_2)) = 0 \) and
\( af(C(P_2,P_4,C_4)) = 1 \).

As special cases of chain graphs, we can consider cactus chains. A cactus graph is a
connected graph in which no edge lies in more than one cycle. Consequently, each block of
a cactus graph is either an edge or a cycle. If all blocks of a cactus \( G \) are cycles of the
same size \( k \), the cactus is \( k \)-uniform. A triangular cactus is a graph whose blocks are
triangles, i.e., a 3-uniform cactus. A vertex shared by two or more triangles is called a cut–
vertex. If each triangle of a triangular cactus \( G \) has at most two cut–vertices, and each cut–
vertex is shared by exactly two triangles, we say that \( G \) is a chain triangular cactus. The
number of triangles in \( G \) is called the length of the chain. An example of a chain triangular
cactus is shown in Figure 3.

![Figure 3: A chain triangular cactus \( T_n \) and square cactus \( O_n \), respectively.](image)

Obviously, all chain triangular cactus of the same length are isomorphic. Hence, we
denote the chain triangular cactus of length \( n \) by \( T_n \), clearly, a chain triangular cactus of
length \( n \) has \( 2n+1 \) vertices and \( 3n \) edges [1]. Since \( T_n \) does not have any perfect
matching, we have \( af(T_n) = 3n \).
By replacing triangles in chain triangular chain $T_n$ by cycles of length 4, we obtain cactus whose every block is $C_4$ as shown in Figure 3. We call such cactus, square cactus and denote a chain square cactus of length $n$ by $O_n$ [1].

**Theorem 2.8** Let $O_n$ be a chain square cactus. We have

I. If $n$ is even, then $af(O_n) = 4n$.

II. If $n$ is odd, then $af(O_n) = \frac{n+1}{2}$.

**Proof.**

I. By Tutte’s Theorem, there is no perfect matching for $O_n$ in this case and so $af(O_n) = 4n$.

II. For this case the anti–forcing number of $O_n$ is equal with the anti–forcing number of $L(C_4, \ldots, C_4)$. Since $af(C_4) = 1$, so we have the result by Theorem 2.4.

This proves the theorem.

3. **Anti–Forcing Number of Some Operations of Graphs**

In this section, we shall study the anti–forcing number of some operations of two graphs. First we consider the join of two graphs. The join $G_1 + G_2$ of graphs $G_1$ and $G_2$ with disjoint point sets $V(G_1)$ and $V(G_2)$ and edge sets $E(G_1)$ and $E(G_2)$ is the graph union $G_1 \cup G_2$ together with all the edges joining $V(G_1)$ and $V(G_2)$. The following theorem gives a lower bound for the anti–forcing of join of two graphs.

**Theorem 3.1** Let $G_1$ and $G_2$ be two simple graphs. Then we have

$$af(G_1 + G_2) \geq af(G_1) + af(G_2).$$

**Proof.** Suppose that $S_1, S_2$ and $S$ have the smallest cardinality over all anti–forcing sets of graphs $G_1, G_2$ and $G_1 + G_2$, respectively. So $af(G_1) = |S_1|$, $af(G_2) = |S_2|$ and $af(G_1 + G_2) = |S|$. By definition of $G_1 + G_2$, $|V(G_1 + G_2)| = |V(G_1)| + |V(G_2)|$ and $|E(G_1 + G_2)| > |E(G_1)| + |E(G_2)|$. Thus for the choosing the perfect matchings of $G_1 + G_2$, we have more possibilities than the number of perfect matching of $G_1$ plus the number of perfect matchings of $G_2$. It means that $|S| \geq |S_1| + |S_2|$ and so we have the result.
Remark 3.2 The lower bound in Theorem 3.1 is sharp. For example \( af(C_3 + C_3) = 6 = af(C_3) + af(C_3) \). Also, if \( G_1 \) is an odd graph and \( G_2 \) is an even graph, then
\[
af(G_1 + G_2) > af(G_1) + af(G_2).
\]
Because for odd graph \( G_1 \), we have \( af(G_1) = |E(G_1)| \) and for even graph \( G_2 \), \( af(G_2) \leq |E(G_2)| \). Also \( G_1 + G_2 \) is an odd graph. So
\[
af(G_1 + G_2) = |E(G_1) + G_2| = |E(G_1)| + |E(G_2)| \geq af(G_1) + af(G_2).
\]
Here, we consider the corona of two graphs and then we study the anti–forcing number of them. We recall that the corona of two graphs \( G_1 \) and \( G_2 \), written as \( G_1 \circ G_2 \), is the graph obtained by taking one copy of \( G_1 \) and \( |V(G_1)| \) copies of \( G_2 \), and then joining the \( i \)-th vertex of \( G_1 \) to every vertex in the \( i \)-th copy of \( G_2 \).

Theorem 3.3 Let \( G_1 \) and \( G_2 \) be two simple graphs. If both of \( G_1 \) and \( G_2 \) have perfect matching, then
\[
af(G_1 \circ G_2) = af(G_1) + |V(G_1)| af(G_2).
\]

Proof. Suppose that \( S_1 \) and \( S_2 \) have the smallest cardinality over all anti–forcing sets of graph \( G_1 \) and \( G_2 \), respectively. So \( af(G_1) = |S_1| \) and \( af(G_2) = |S_2| \). Let \( V(G_1) = \{x_1, x_2, \ldots, x_n\} \) and \( V(G_2) = \{y_1, y_2, \ldots, y_m\} \). For every \( 1 \leq i \leq n \) and every \( 1 \leq j \leq m \), the edge \( x_i y_j \) cannot be in the perfect matchings of \( G_1 \circ G_2 \). Let \( S \) has the smallest cardinality over all anti–forcing sets of graph \( G_1 \circ G_2 \). Then
\[
S = S_1 \cup S_2 \cup \ldots \cup S_2
\]
and we have
\[
af(G_1 \circ G_2) = |S| = |S_1| + |V(G_1)| |S_2| \leq af(G_1) + |V(G_1)| af(G_2).
\]
This completes the proof. 

Clearly, If \( G_1 \) has a unique perfect matching, then \( af(G_1 \circ G_2) = |V(G_1)| af(G_2) \) and if \( G_2 \) has a unique perfect matching, then \( af(G_1 \circ G_2) = af(G_1) \). For example \( af(C_4 \circ P_2) = 1 \) and \( af(P_2 \circ C_4) = 2 \).

Now this question comes to mind: what happens to the anti–forcing number of graph \( G_1 \circ G_2 \), when at least one of the \( G_1 \) or \( G_2 \) does not have any perfect matching? It can easily verified that if only \( G_1 \) does not have any perfect matching, then the graph \( G_1 \circ G_2 \) does not have any perfect matching too and so \( af(G_1 \circ G_2) = |E(G_1 \circ G_2)| \). But if \( G_2 \) does not have perfect matching, then the anti–forcing number of \( G_1 \circ G_2 \) just depends on \( G_2 \), because assume that \( u \in V(G_1) \) and \( (G_2) \), be a copy of \( G_2 \) such that the vertex \( u \) is adjacent to every
vertex of $(G_2)_u$. Since $G_2$ does not have any perfect matching, then it has at least one unsaturated vertex. Without loss of generality we can suppose that $v \in V((G_2)_u)$ is the unsaturated vertex of $(G_2)_u$. Then $uv \in M$ where $M$ is a maximum matching of graph $G_1 \circ G_2$. Thus every vertex of $G_1$ in $M$ is saturated by the edges that connect $G_1$ with $G_2$. In the following propositions, we consider the anti–forcing number of $G_1 \circ G_2$, when $G_2$ is a path, cycle or wheel of odd order $n$, respectively.

**Figure 4:** The $K_1 \circ P_n$ in the proof of Proposition 3.4.

**Proposition 3.4** Let $G$ be a simple graph and $P_n$ a path of odd order $n$. We have

$$af(G \circ P_n) = |V(G)|.$$

**Proof.** Let $u \in V(G)$ and $(P_n)_u$ be a copy of $P_n$ with the vertex set $\{v_1, \ldots, v_n\}$ such that the vertex $u$ is adjacent to all vertices of $(P_n)_u$. It can easily verified that if $v$ is one of the vertices in the set $\{v_1, v_3, \ldots, v_{n}\}$, then the edge $uv$ belongs to a perfect matching of graph $G \circ P_n$. Since $P_n - v$ has unique perfect matching and there exist $(n+1)/2$ ways to choose vertex $v \in V(P_n)$, so we can conclude that the number of perfect matchings of $K_1 \circ P_n$ is equal to $(n+1)/2$. Also $n$ is odd and so the perfect matching of $G \circ P_n$ does not related to the perfect matching of $G$. Thus the number of perfect matchings of $G \circ P_n$ is equal to $[(n+1)/2]^{|V(G)|}$. Let $S = \{e_1\}$ (see Figure 4). Then $S$ has the smallest cardinality over all anti–forcing sets of graph $K_1 \circ P_n$. So for each odd $n$, we have $af(K_1 \circ P_n) = 1$. Obviously, the number of graphs $K_1 \circ P_n$ is equal to $|V(G)|$ and this implies the result.  

**Proposition 3.5** Let $G$ be a simple graph and $C_n$ be a cycle of odd order $n$. We have

$$af(G \circ C_n) = 2|V(G)|.$$

**Proof.** Let $u \in V(G)$ and $(C_n)_u$ be a copy of $C_n$ such that the vertex $u$ is adjacent to every vertex of $(C_n)_u$. Suppose that $v \in V((C_n)_u)$ and $uv$ belongs to one of the perfect matchings
of graph $G \circ C_n$. Since $C_n - v = P_{n-1}$, so $C_n - v$ has an unique perfect matching. Also to choose vertex $v \in V(C_n)$ we have $n$ possibilities. Note that since $n$ is odd, thus the perfect matching of $G \circ C_n$ does not related to the perfect matching of $G$ and we can conclude that the number of perfect matchings of $G \circ C_n$ is equal to $n^{\left| V(G) \right|}$. Let $S = \{e_1, e_2\}$ be as shown in Figure 5. Clearly, $S$ has the smallest cardinality over all anti--forcing sets of graph $K_1 \circ C_n$. So for every odd $n$, we have $af(K_1 \circ C_n) = 2$. Also the number of graphs $K_1 \circ C_n$ is equal to $\left| V(G) \right|$. So we have the result.

![Figure 5](image)

**Figure 5:** The graph with $S = \{e_1, e_2\}$ in the proof of Proposition 3.5.

**Proposition 3.6** Let $G$ be a simple graph and $W_n$ a wheel of odd order $n$. We have

$$af(G \circ W_n) = 4\left| V(G) \right|.$$  

**Proof.** Let $u \in V(G)$ and $(W_n)_u$ be a copy of $W_n$ such that $u$ is adjacent to every vertex of $(W_n)_u$. Suppose that $v \in V((W_n)_u)$ and $uv$ belongs to one of the perfect matchings of graph $G \circ W_n$. If $v \in C_{n-1}$, then to choose other edges of perfect matching of $K_1 \circ W_n$, we have $(n-1)/2$ possibilities and if $v \in K_1$, then there exist two possibilities to choose other edges of perfect matching of $K_1 \circ W_n$. Since $n$ is odd, so the perfect matching of $G \circ W_n$ does not related to the perfect matching of $G$. Also $C_{n-1}$ have $n-1$ vertices. Thus to choose perfect matching of $G \circ W_n$, we have $\left[ 1/2(n-1)^2 + 2 \right]^{\left| V(G) \right|}$ possibilities. Let $S = \{e_1, e_2, e_3, e_4\}$ as shown in Figure 6. Observe that $S$ has the smallest cardinality over all anti--forcing sets of graph $K_1 \circ W_n$. Then for every odd $n$, $af(K_1 \circ W_n) = |S| = 4$ and we can conclude that $af(G \circ W_n) = 4\left| V(G) \right|$.  

4. Anti-Forcing Number of Some Dendrimers

Dendrimers are hyper-branched macromolecules, with a rigorously tailored architecture. They can be synthesized, in a controlled manner, either by a divergent or a convergent procedure. Dendrimers have gained a wide range of applications in supra-molecular chemistry, particularly in host guest reactions and self-assembly processes. Their applications in chemistry, biology and nano-science are unlimited [2].

In this section, we shall find the anti–forcing number of certain polyphenylene dendrimers. First we obtain the anti–forcing number of the first kind of dendrimer of generation 1–3 that has grown $n$ stages. We denote this graph by $D_3[n]$. Figure 7 shows the first kind of dendrimer of generation 1–3 has grown 3 stages $D_3[n]$. Also we shall study the anti–forcing number of the first kind of dendrimer which has grown $n$ steps denoted $D_1[n]$. Figure 7 shows $D_1[4]$. Note that there are three edges between each two cycle $C_6$ in this dendrimer.

Theorem 4.1

(i) Let $D_3[n]$ be a kind of dendrimer of generation 1–3 that has grown $n$ stages. Then $af(D_3[n]) = 3 \times 2^{n+4} - 24$.

(ii) Let $D_1[n]$ be a kind of dendrimer that has grown $n$ stages. Then $af(D_1[n]) = 9 \times 2^{n+1} - 11$.

Proof.

(i) It follows from Tutte’s Theorem.

(ii) It can be observe that from Figure 7 that $D_1[n]$ is an odd graph. So $af(D_1[n]) = |E(D_1[n])| = 25 + \sum_{i=1}^{n-1} (18 \times 2^i)$. 

Figure 6: The graph with $S = \{e_1, e_2, e_3, e_4\}$ in the proof of Proposition 3.6.
This completes our argument.

Figure 7: The dendrimers $D_3[3]$ and $D_4[4]$, respectively.

Finally we consider another type of polyphenylene dendrimer by construction of dendrimer generations $G_n$ that has grown $n$ stages. We simply denote this graph by $PD_2[n]$. Figure 8 shows the generations $G_3$ that has grown 3 stages.

**Theorem 4.2** Let $PD_2[n]$ be a type of polyphenylene dendrimer by construction of dendrimer generations $G_n$ that has grown $n$ stages. Then we have

$$af(PD_2[n]) = 2 + \sum_{i=1}^{n} (5 \times 2^{i+1}).$$

**Proof.** As you see in Figure 8,

$$PD_2[n] = L(\underbrace{C_6, C_6, \ldots, C_6}_{(2+\sum_{i=1}^{n} 5 \times 2^{i+1})-times}).$$

Now the result follows from Theorems 2.1 and 2.4.
Figure 8: Polyphenylene dendrimer of generations $G_3$ that has grown 3 stages.

ACKNOWLEDGEMENTS. The authors would like to express their gratitude to the referees for their careful reading and helpful comments.

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