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Global forcing number of benzenoid graphs

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A global forcing set in a simple connected graph G with a perfect matching is any subset S of $E(G)$ such that the restriction of the characteristic function of perfect matchings of G on S is an injection. The number of edges in a global forcing set of the smallest cardinality is called the global forcing number of G. In this paper we prove several results concerning global forcing sets and numbers of benzenoid graphs. In particular, we prove 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.

KEY WORDS: global forcing number, benzenoid graph

1. Introduction and motivation

Forcing sets and forcing numbers are just two of many graph-theoretical concepts that can trace their origin back to the study of resonance structures in mathematical chemistry [8,9]. Both of them later attracted considerable interest in purely graph-theoretical literature [1,2,11,12,18]. Common to all those works was the local approach to the forcing sets and numbers: forcing sets were defined with respect to particular perfect matchings, and global invariants were derived by taking minimum over all perfect matchings in the graph. In this paper, we get back to the chemical roots of forcing-related concepts, but we define them globally, i.e., without reference to a particular perfect matching. Global forcing sets have been already introduced and studied for certain classes of graphs in refs. [14,17]. The motivation for their study comes from rather large-scale computations involving manipulation of perfect matchings in fullerene graphs [15, 16], since global forcing sets can serve as binary codes for perfect matchings.

The present paper is organized as follows. In the next section, we introduce and formally define global forcing sets and numbers, along with other graph-theoretic terms relevant for our subject. The same section contains some auxiliary results valid for general graphs with perfect matchings. In section 3, we specialize those results on catacondensed benzenoids and other catacondensed

polymers made of even cycles and prove explicit formulas for their global forcing numbers. Section 4 is concerned with pericondensed benzenoids, both normal and essentially disconnected. We provide lower and upper bounds on the global forcing number of such graphs. The last section is devoted to catafused coronoids, where we again prove an explicit formula for their global forcing numbers. Some possible directions of future research are briefly discussed at the end.

2. Definitions and auxiliary results

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 [10].

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 called *normal*. For connected bipartite graphs, the elementarity is equivalent to the property that all edges are allowed ([10], p. 122).

Let $G = (V(G), E(G))$ be a graph with a perfect matching. Denote by $\mathcal{M}(G)$ the set of all perfect matchings in G and by f the characteristic function of perfect matchings of G, i.e., the function $f : \mathcal{M}(G) \to \{0, 1\}^{|E(G)|}$ defined by

$$[f(M)]_i = \begin{cases} 1, & e_i \in M, \\ 0, & e_i \notin M. \end{cases}$$

Any set $S \subseteq E(G)$ such that the restriction of f on S is an injection is called a *global forcing set* of G. A global forcing set of the smallest cardinality is called a *minimal global forcing set*, and its cardinality is the *global forcing number* of G. For a given graph G we denote this quantity by $\gamma(G)$.

For a given perfect matching $M \in \mathcal{M}(G)$, the value $f(M)$ is, in fact, a code of M in the binary alphabet. This fact gives us a lower bound on the invariant $\gamma(G)$ in terms of the number of perfect matchings in G. Namely, if a given graph G has $K(G)$ perfect matchings, we need at least $\lceil \log_2 K(G) \rceil$ binary digits for representing those perfect matchings as distinct binary numbers. Hence, we have established the following result.

Proposition 1. Let G be a graph with $K(G)$ perfect matchings. Then $\gamma(G) \geqslant \lceil \log_2 K(G) \rceil$.

We can further emphasize the "logarithmic" behavior of $\gamma(G)$ by putting $\gamma(G) = 0$ if G has unique perfect matching, and even by defining $\gamma(G) = -\infty$ for graphs without perfect matchings.

The main problem with the bound from proposition 1 is that the quantity $K(G)$ is, in general, difficult to express in terms of the basic graph parameters, such as the number of vertices and/or edges. Explicit formulas are only rarely available, and $K(G)$ can be NP-hard to compute even for bipartite graphs ([10], p. 307). Hence, it makes sense to search for more direct relations connecting $\gamma(G)$ and the graph size. The following results are useful stepping stones in that direction.

We start by observing that an edge appearing in no perfect matching of G carries no information about $\gamma(G)$, and that any global forcing set containing such edges cannot be minimal. Hence, the set of forbidden edges can be removed from G before considering the global forcing in G.

Lemma 2. Let G be a simple connected graph with perfect matchings and F the set of forbidden edges in G. Then $\gamma(G) = \gamma(G - F)$.

Lemma 3. Let G be a simple connected graph with perfect matchings and S a minimal global forcing set. Then $G - S$ is a spanning subgraph of G.

Proof. Let us suppose that the claim is not true. Then there must be a vertex $v \in V(G)$ such that no edge of $G - S$ is incident with v. It means that all edges incident with v are in S. Let us denote those edges by $e_1, \ldots, e_k$. If $k > 1$, the vector $f|_{\{e_1,\ldots,e_k\}}$ has exactly one component equal to 1, all others being 0. Let this component be the one corresponding to e_1. But then the edges $e_2, \ldots, e_k$ appear in no perfect matching of G, i.e., they are forbidden. Their removal from S would then result in a global forcing set of a cardinality smaller than $|S|$, a contradiction. If $k = 1$, then e_1 is in every perfect matching of G, and its presence in S carries no information. Hence, it can be deleted from S, and the set $S - e$ will still be a global forcing set, again a contradiction. □

From lemma 3 we have the following upper bound on $\gamma(G)$.

Proposition 4. Let G be a simple connected graph with a perfect matching. Then $\gamma(G) \leqslant |E(G)| - |V(G)| + 1$.

Proof. Let T be a spanning tree of G. The set $E(G) - E(T)$ contains $|E(G)| - |V(G)| + 1$ edges. If $E(G) - E(T)$ is not a global forcing set, then there must be two perfect matchings $M_1 \neq M_2$ of G that coincide on $E(G) - E(T)$. Their symmetric difference $M_1 \Delta M_2$ then must contain at least one alternating cycle, and the edges of that cycle are not in $E(G) - E(T)$. But they cannot be in $E(T)$ either, since T is a tree, and we have a contradiction. Hence, $E(G) - E(T)$ is a global forcing set, and $\gamma(G) \leqslant |E(G)| - |V(G)| + 1$. □

The same argument in a bit more general setting yields the following characterization of global forcing sets.

Proposition 5. Let G be a simple connected graph with a perfect matching. A set $S \subseteq E(G)$ is a global forcing set if and only if the graph induced by $E(G) - S$ has at most one perfect matching.

From the proof of proposition 4 one can see that the presence of even cycles in $E(G) - S$ is the main obstacle to a set S being a global forcing set. An even cycle C in $E(G) - S$ is permitted only if the graph induced by the vertices that remain after deleting the vertices of C contains no perfect matchings. This observation also yields the class of graphs for which the upper bound of proposition 4 is sharp.

A subgraph $H \subseteq G$ is *nice* if $G - H$ contains a perfect matching. Using the concept of nice even cycles will simplify the formulation and proof of the following result.

Proposition 6. Let G be a simple connected bipartite graph with a perfect matching. Then $\gamma(G) = |E(G)| - |V(G)| + 1$ if and only if all even cycles in G are nice.

Proof. Let G be a bipartite graph such that every (even) cycle is nice. Then no even cycle may be contained in $G - S$, where S is a global forcing set. As the bipartite graphs contain only even cycles, it means that $G - S$ contains no cycles at all. Since we are interested in global forcing sets of the smallest cardinality, we must look for acyclic subgraphs of G with the largest possible number of edges, i.e., for spanning trees. The claim now follows by subtracting the number of edges in a spanning tree from the total number of edges of G.

Let G now be a bipartite graph and $C \subseteq E(G)$ an even cycle that is not nice. Let e be an edge of C, and P the path on an even number of vertices obtained from C by deleting the edge e. Let T_C be any spanning tree of G that contains P as an induced subgraph. The set of edges $S_C = E(G) - E(T)$ is a global forcing set, since T has at most one perfect matching. Moreover, $e \in S_C$. Define the set S by $S = S_C - e$. We claim that S is also a global forcing set. Let $M_1 \neq M_2$ be two perfect matchings of G that coincide on S. Then their symmetric difference $M_1 \Delta M_2$ contains an alternating cycle in $G - S = T_C \cup \{e\}$. But the only even cycle in $G - S$ is the cycle C. Since the graph induced by $V(G) - V(C)$ contains no perfect matchings, neither M_1 nor M_2 can be extended to a perfect matching of G, a contradiction. Hence, any two perfect matchings that coincide on S must coincide on G, and S is a global forcing set. Since $|S|$ is strictly smaller than $|S_C| = |E(G)| - |V(G)| + 1$, the claim follows. □

3. Catacondensed benzenoids

Let us now consider the main subject of the present paper, the benzenoid graphs. A *benzenoid system* is a one-connected collection of congruent regular hexagons arranged in the plane in such a way that any two hexagons that have a common point intersect in a whole edge. From the conditions of regularity and congruence it follows that benzenoid systems are subsets (with one-connected interior) of a regular tiling of the plane by hexagonal tiles. To each benzenoid system we assign a graph, taking the vertices of hexagons as the vertices of the graph, and the sides of hexagons as the edges of the graph. The resulting *benzenoid graph* is simple, plane, and bipartite. The vertices lying on the border of the unbounded face of a benzenoid graph are called *external*; other vertices, if present, are called *internal*. A benzenoid graph without internal vertices is *catacondensed*. Otherwise, the graph is *pericondensed*. In the rest of the paper, when referring to benzenoids, we will be referring to the corresponding benzenoid graphs.

Perfect matchings in benzenoid graphs are known in the chemical literature as *Kekulé structures*, and the benzenoids possessing them are called *Kekuléan*. For more information on benzenoid graphs, and in particular for a review of results concerning the enumeration of perfect matchings in them, we refer the reader to the monograph [4].

After the groundwork in the previous section, most of our results concerning the benzenoid graphs will follow almost at a glance. We treat the catacondensed case first.

It is well known that all catacondensed benzenoids are Kekuléan and elementary [4]. Further, the number of Kekulé structures in a catacondensed benzenoid can vary from a linear (as in a linear polyacene) to an exponential function of the number of hexagons (as in nowhere-straight unbranched chains of hexagons). Moreover, empiric results indicate that for a given number of hexagons, the highest Kekulé structure count is invariably attained for a catacondensed benzenoid [3]. Taking all this into account, it is quite surprising, in view of proposition 1, that the global forcing number of a catacondensed benzenoid depends only on its number of hexagons.

Proposition 7. Let B_n be a catacondensed benzenoid with n hexagons. Then $\gamma(B_n) = n$.

Proof. Let C be an even cycle in a catacondensed benzenoid B_n with n hexagons. The graph induced by $V(B_n) - V(C)$ has certain number of components, and each of them is of the form shown in figure 1. Here $m \geqslant 0$ and CB_1 and CB_2 denote some smaller catacondensed benzenoids; they may also be empty. (If $m = 0$, then necessary both CB_1 and CB_2 must be empty.) It is easy to see that each such component has a perfect matching, and their union is a perfect

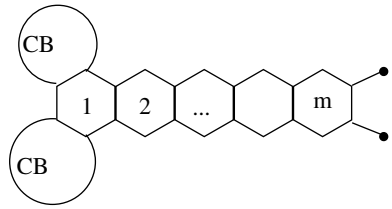

Figure 1. A component of $B_n - V(C)$.

matching in $B_n - V(C)$. Hence, every even cycle in B_n is nice, and the claim now follows by proposition 6. □

By combining propositions 1 and 7 we get an upper bound on the number of perfect matchings in catacondensed benzenoids with n hexagons.

Corollary 8. Let B_n be a catacondensed benzenoid with n hexagons. Then $K(B_n) \leqslant 2^n$.

The result of proposition 7 remains valid if instead of hexagons we allow other even cycles as the basic building blocks of a catacondensed polymer. The only difference is that in the proof, in order to avoid case-by-case analysis, we rely on the ear decomposition technique for elementary bipartite graphs. We refer the reader to chapter 4 of [10] for a comprehensive treatment of the ear decomposition method, or to [5, 6] for some chemically relevant applications.

Corollary 9. Let G_n be a catacondensed polymer made of n even cycles. Then $\gamma(B_n) = n$.

Proof. Again, we consider an even cycle C in G_n. We want to show that C is nice. If $V(C) = V(G_n)$, it follows by definition. If C is not a spanning subgraph of G_n, then all the remaining vertices can be added to C as *ears*, i.e., as odd-length paths, one at a time. Since each ear possesses a perfect matching, the union of those matchings is a perfect matching in $G_n - V(C)$, and the claim follows by proposition 6. □

Chemically interesting examples of such catacondensed polymers are, e.g., phenyllenes.

4. Pericondensed benzenoids

We consider here only the pericondensed benzenoids with perfect matchings, i.e., only the Kekuléan ones. Unlike the catacondensed benzenoids, Kekuléan pericondensed benzenoids may contain forbidden edges. Pericondensed

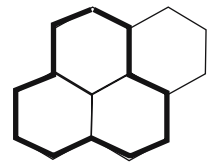

Figure 2. Graph $B_{2,2}$ that is subgraph of all normal benzenoids.

benzenoids without forbidden edges are called *normal*; those with forbidden edges are called *essentially disconnected*. The term is justified by the fact that a removal of forbidden edges results in a disconnected graph consisting of normal components.

The following result for normal benzenoids is a direct consequence of proposition 6.

Proposition 10. Let N_n be a normal pericondensed benzenoid with n hexagons. Then $\gamma(N_n) \leqslant n - 1$.

Proof. The graph $B_{2,2}$ shown in figure 2 is contained as an induced subgraph in all normal pericondensed benzenoids. Obviously, the even cycle shown in bold in figure 2 is not nice. Then, by proposition 6, we have $\gamma(N_n) < |E(N_n)| - |V(N_n)| + 1$, and the claim follows by application of the Euler formula. □

The graph $B_{2,2}$ is also an example of a normal pericondensed benzenoid with n hexagons for which the upper bound $\gamma(N_n) \leqslant n - 1$ is actually attained. Namely, from proposition 10 we have $\gamma(B_{2,2}) \leqslant 3$, and since $K(B_{2,2}) = 6$, from proposition 1 we have $\gamma(B_{2,2}) \geqslant 3$. It is quite possible that $B_{2,2}$ and the graphs obtained from $B_{2,2}$ by appending catacondensed benzenoids to it without creating new internal vertices are the only normal pericondensed benzenoids with $\gamma(N_n) = n - 1$. A plausible explanation would be that the other non-nice even cycles will further reduce the upper bound on $\gamma(N_n)$, but the details still need to be worked out.

Let us now turn our attention to the essentially disconnected benzenoids. When all normal components of such a graph are catacondensed, we can use the previous results to derive the following bounds on the global forcing number.

Proposition 11. Let D_n be an essentially disconnected benzenoid with n hexagons whose normal components $C_1, \ldots, C_l$ are all catacondensed. Then $\gamma(D_n) = \sum_{i=1}^{l} \gamma(C_i)$. In particular, $l + 2 \leqslant \gamma(D_n) \leqslant n - l + 1$.

Proof. Formula $\gamma(D_n) = \sum_{i=1}^{l} \gamma(C_i)$ follows from proposition 2 and the fact that the global forcing number of a disconnected graphs is equal to the sum of global forcing numbers of its connected components.

The lower bound $l + 2 \leqslant \gamma(D_n)$ follows from a result proven in [13] that, if an essentially disconnected benzenoid has l normal components, then at most $l - 2$ of them can be single hexagons. As each single hexagon contributes 1 to $\gamma(D_n)$, the lower bound is established. The upper bound follows from the fact that all l normal components together cannot have more than $n - l + 1$ hexagons. □

Both the upper and lower bound of proposition 11 are sharp. The extremal graphs are shown in figure 3. If we drop the condition that all normal components be catacondensed, the bounds of proposition 11 are weakened. Even with catacondensed normal components the gap between the bounds of proposition 11 and the actual values can be arbitrarily large, as can be seen from the examples shown in figure 4. For the left graph we have $\gamma(G) = 4$; for the right one, $\gamma(G) = n - 1$. The number 4 is in no way special, since for each $k \geqslant 4$ we can construct an essentially disconnected benzenoid with $\gamma(D_n) = k$ and $n \geqslant k + 1$ arbitrarily large. For more details, the reader might consult [7].

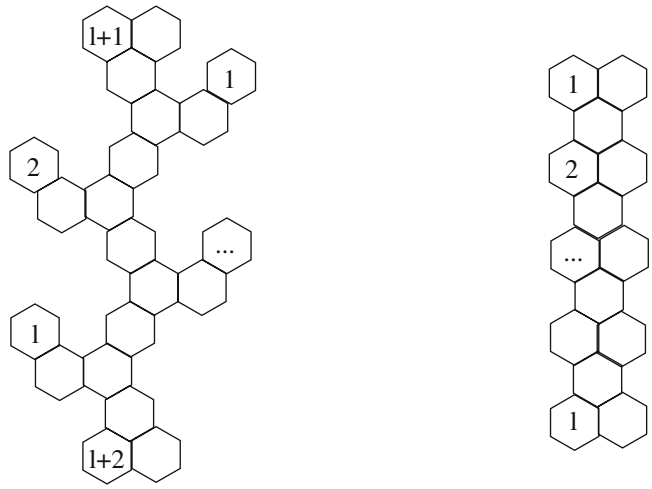

Figure 3. Essentially disconnected benzenoids extremal with respect to $\gamma(G)$.

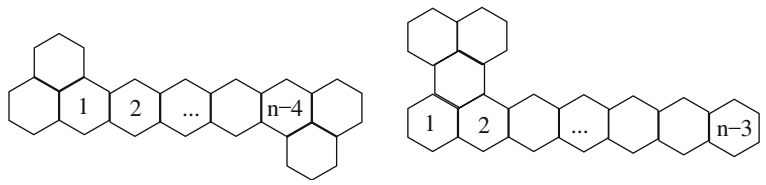

Figure 4. Essentially disconnected benzenoids with arbitrarily large gaps between bounds and actual values for $\gamma(G)$.

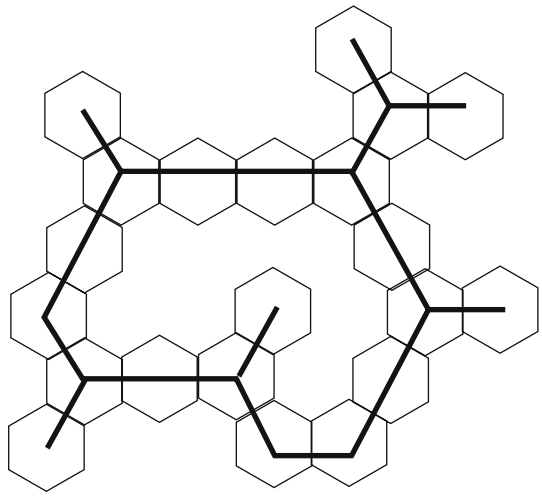

Figure 5. A catafused coronoid and its inner dual.

5. Catafused coronoids

In this section, we consider global forcing sets and numbers of certain coronoid graphs. By a *coronoid graph* we mean a graph obtained from a pericondensed benzenoid by deleting some internal vertices and/or edges in such a way that no remaining vertex is of degree one, there is only one bounded non-hexagonal face, and this face is not adjacent to the unbounded face of the graph. Such graphs are not benzenoids in the strict sense, and many results valid for benzenoids break down for coronoids. However, there are enough similarities to justify considering them here.

We restrict our attention to *catafused coronoids*. A coronoid graph is catafused if it has no vertices shared between three hexagons. Equivalently, a coronoid is catafused if its inner dual is a unicyclic graph. (An *inner dual* of a benzenoid graph is obtained from its standard dual by deleting the vertex corresponding to the unbounded face and all incident edges. In the coronoid case, we delete also the vertex corresponding to the bounded non-hexagonal face and the incident edges.) An example of a catafused coronoid is shown in figure 5, together with its inner dual.

Like the catacondensed benzenoids, catafused coronoids do not have internal vertices. This means that their inner duals are triangle-free. Another similarity is that all catafused coronoids are Kekuléan and elementary.

Proposition 12. Let CC_n be a catafused coronoid with n hexagons. Then CC_n is Kekuléan, all edges of CC_n are allowed, and $K(CC_n) \geqslant n + 2$.

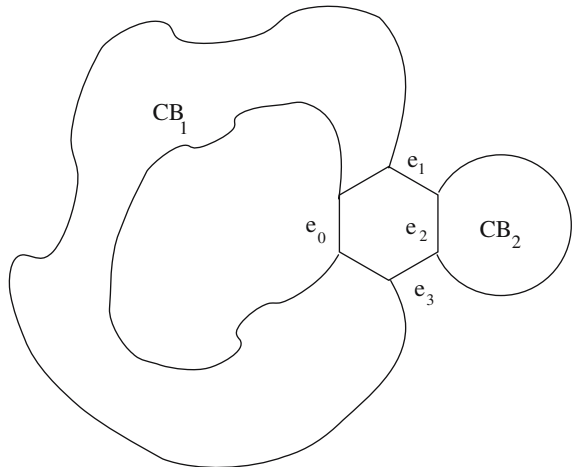

Figure 6. A key hexagon in a catafused coronoid.

Proof. We start by observing that in every catafused coronoid there must be a hexagon of the type shown in figure 6. In fact, there must be at least six such hexagons, but one will suffice here. We call such a hexagon a *key hexagon*. In figure 6, CB_1 and CB_2 denote two catacondensed benzenoids, and we assume that CB_1 is not empty. The catacondensed benzenoid CB_1 can be constructed by the ear decomposition technique. By adding first e_0 as a single-edge ear, and then the three-edge ear $\{e_1, e_2, e_3\}$, we obtain a graph that is still bipartite and elementary. If the catacondensed benzenoid CB_2 is not empty, it can be added to the already constructed graph one hexagon (i.e., one ear) at a time, preserving all the way the property of being bipartite and elementary. Hence, the whole CC_n is bipartite and elementary, and the lower bound follows from the structural theory of matchings ([10], p. 294). □

The difference between the elementarity of catacondensed benzenoids and catafused coronoids is that in catacondensed benzenoids every even cycle is nice, while in catafused coronoids this is not true. In fact, in every catafused coronoid there is an even cycle that is not nice. This fact will be instrumental in establishing one half of the following result.

Proposition 13. Let CC_n be a catafused coronoid with n hexagons. Then $\gamma(CC_n) = n$.

Proof. We first prove that in every catafused coronoid CC_n there is an even cycle that is not nice. The main role in the proof will be played by the hexagons that correspond to the vertices of the unique cycle in the inner dual. Those hexagons form a ring in CC_n that we call the *main ring*.

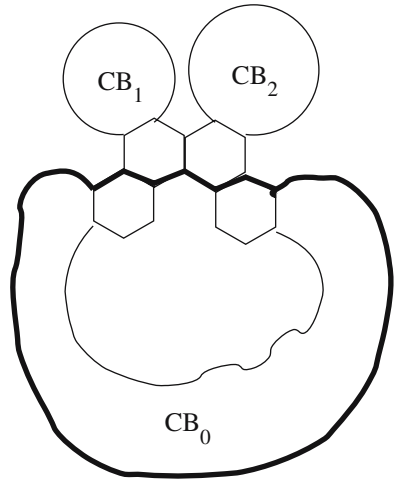

Figure 7. Catafused coronoid whose main ring is made of key hexagons only.

If the main ring contains a hexagon that is not a key hexagon, then one vertex of this hexagon is on the border of the unbounded face of CC_n, and another one is on the border of the bounded non-hexagonal face of CC_n. As those two vertices are non-adjacent, it is clear that the even cycle spanned by all other vertices of CC_n cannot be nice.

Let us suppose that the main ring contains only key hexagons. Then there must be a configuration shown in figure 7. Here the catacondensed benzenoid CB_0 is not empty, while CB_1 and/or CB_2 may be empty. Then the even cycle shown in bold in figure 7 cannot be nice. Hence, in every catafused coronoid there is a non-nice even cycle, and this, by proposition 6, implies that $\gamma(CC_n) \leqslant n$. The claim of the proposition will follow if we prove that no set containing fewer than n edges can be a global forcing set. We model the proof after [14].

It is easy to see that the set of $n-1$ edges that are shared by two hexagons (so called inner edges) cannot be a global forcing set, since it does not force any of four perfect matchings that contain only peripheral edges, i.e., the edges from two even cycles that serve as the borders of two non-hexagonal faces of CC_n. Let us now suppose that there is a global forcing set T of $n-1$ edges, some of them inner, some peripheral. Now switch to the inner dual. For each inner edge in T we mark the corresponding edge in the inner dual; for each hexagon that contains a peripheral edge of T, we mark the corresponding vertex. Let x denote the number of marked vertices and y the number of marked edges. Then $x+y \leqslant |T| \leqslant n-1$, since a hexagon may contain more than one peripheral edge from T. Now delete all marked vertices and unmarked edges from the inner dual. The remaining graph has $n-x$ vertices and y edges. Since $n-x \geqslant y+1$, the remaining graph must contain at least one non-empty component. This component has

$k \geqslant 1$ vertices, and it is either a tree, or a smaller unicyclic graph. If it is a tree, it corresponds to a catacondensed benzenoid of k hexagons that are collectively incident with $k-1$ edges of T, and we already know that such set of edges cannot be a global forcing set in a catacondensed benzenoid. If the component is a unicyclic graph, it corresponds to a catafused coronoid on k hexagons that are collectively incident with exactly k edges of T, all of them inner. But we have already showed that such a set of edges cannot be a global forcing set of catafused coronoid, and hence T cannot be a global forcing set in CC_n. So, a minimal global forcing set in CC_n must have at least n edges, and this proves the claim. □

We conclude the paper by some open problems and conjectures. The cases of catacondensed benzenoids and catafused coronoids are completely settled here. For the essentially disconnected pericondensed benzenoids we have also obtained a fair number of results. However, the normal pericondensed benzenoids are barely scratched on the surface, and it would be interesting to learn more about forcing sets and numbers in such graphs. For example, one could try to characterize the normal benzenoids for which the upper bound of proposition 10 is attained, or to explore how large the gap can be. Further, it would be useful to determine exactly the global forcing numbers of benzenoid parallelograms and other simple subsets of hexagonal grids after the pattern of Ref. [14]. The most promising approach seems to be via counting non-nice even cycles, but the details are far from clear.

One could also go beyond the catafused coronoids by considering the *catafused reticulenes*. They are formed according to the same rules as the coronoids, but may have several bounded non-hexagonal faces. We believe that the global forcing number of a catafused reticulene $R_{n,m}$ with n hexagonal and m non-hexagonal bounded faces is given by formula $\gamma(R_{n,m}) = n - m + 1$.

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