FORCING INDEPENDENCE

CRAIG LARSON AND NICO VAN CLEEMPUT

Abstract. An *independent set* in a graph is a set of vertices which are pairwise non-adjacent. An independent set of vertices F is a *forcing independent set* if there is a unique maximum independent set I such that $F \subseteq I$. The *forcing independence number* or *forcing number* of a maximum independent set I is the cardinality of a minimum forcing set for I. The forcing number f of a graph is the minimum cardinality of the forcing numbers for the maximum independent sets of the graph. The possible values of f are determined and characterized. We investigate connections between these concepts, other structural concepts, and chemical applications.

Keywords. Forcing, independent set, independence number, benzenoids.

1. Dedication

The authors dedicate this article to Prof Douglas Klein on occasion of his 70^{th} birthday. Doug is a passionate scientist, ebullient educator, tireless worker, and generous supporter—and a role model for all young scientists. He is overflowing with knowledge, history, and ideas—and eager to share them. The first author had the privilege of spending six months with Doug in Galveston in 2012, where he heard lots of interesting mathematics and chemistry, and tools and techniques, which he hopes to master.

2. Introduction

An *independent set* in a graph is a set of vertices which are pairwise non-adjacent, that is, a set of vertices with no edges between them. This concept appears in a variety of chemical contexts, though its full significance is not yet understood. Finding a maximum independent set is a well-known widely-studied NP-hard problem. The problem of finding a maximum independent set in a graph appears in a number of practical contexts including, for instance, in measuring the complexity of sending error-free messages.[1] We will describe minimal sets which, in some sense, describe the long-range independence structure of a graph. For instance, the identification

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of no more than one vertex of "small" benzenoids identifies the unique maximum independent set containing that vertex (see Figs. 5 and 7).

An independent set of vertices F is a *forcing independent set* (or *forcing set*) if there is a unique maximum independent set I such that $F \subseteq I$. This concept parallels a concept defined for matchings by Randić and Klein. We investigate connections between forcing independent sets and other structural concepts. For instance, if a graph has a unique maximum independent set, then $F = \emptyset$ is a forcing set. It will also be seen that the complement of a forcing set together with its neighbors induces a graph which has a unique maximum independent set. So there is a strong connection between forcing independent sets and the theory of unique maximum independent sets.[2–4]

2.1. **Forcing Matching.** A *matching* in a graph is a set of independent edges, that is, a set of edges which have no vertices in common. If these edges saturate the vertices of the graph then the graph has a *perfect matching* or *Kekulé structure*. Randić and Klein define the *degree of freedom df* of a Kekulé structure M to be the cardinality of a minimum set of independent edges F so that M is the unique Kekulé structure with $F \subseteq M$.[5] They show that molecular resonance energy of a sample of benzenoids correlates strongly with the log of the sum of the degrees of freedom of the molecule's Kekulé structures. In the sequel Klein and Randić compare *df* to other Kekulé structure-based invariants.[6] More recently Vukičević, Kroto, and Randić use *df* as a way to systematize their atlas of the Kekulé structures of Buckminsterfullerene C_{60}.[7]

Harary, Klein and Zivkovic define the *forcing number* of a matching in a way equivalent to the definition of the degree of freedom of the matching.[8] Among other things, they give an algorithm to calculate it for benzenoids. The authors suggest here that forcing independence would also be of interest. Klein and Rosenfeld have generalized the notion of forcing sets of Kekulé structures to other covering structures.[9] Zhang, Ye, and Shiu have found lower bounds for the forcing matching number of fullerenes.[10] Vukičević and Trinajstić have investigated the *anti-forcing* number of benzenoids, the smallest number of edges that must be removed from a benzenoid so that a single Kekulé structure remains.[11]

2.2. **Independence in Chemistry.** Matching theory, beginning with the identification of the significance of Kekulé structures, has a long history of chemical application. Independence theory has direct relationships with matching theory—but its utility in chemistry is less clear.

In an *alternant* (or *bipartite*) hydrocarbon, such as the family of benzenoids, one rule-of-thumb in discussing their stability is that species with paired carbon electrons will be more stable than species with free electrons. This is only a first approximation, as isomers with paired carbon electrons are not equally stable, and species with unpaired electrons can be stable. Nevertheless, this rule-of-thumb implies that the graph of a stable alternant hydrocarbon will have a perfect matching and, thus, that the matching number ν will be half the number of vertices.

The König-Egerváry Theorem[12] guarantees that, in a bipartite graph, $\alpha+\nu = n$. Thus for bipartite graphs, the matching number and independence number are complementary invariants, where a value for one gives the value for the other. The independence number α of an alternant hydrocarbon where all carbon electrons are paired is half the number of atoms; for any alternant hydrocarbon with unpaired carbon electrons, the independence number is necessarily more than half the number of atoms.

The number of Kekulé structures in a molecule is one factor in molecular stability (Schamlz, *et al.*,[13] for instance, found that there are $12,500$ of these in stable Buckminsterfullerene C_{60}). Merrifield and Simons show that the number σ of independent sets in the graph of the alkane C_nH_{2n+2} correlates with the heat of formation—at least for small values of n.[14] They also show that σ correlates with the boiling points of these alkanes.

Fowler and his collaborators show that the experimentally realized structure of $C_{60}Br_{24}$ can be predicted from $300,436,595,453,640$ mathematically possible brominated fullerene structures.[15] One of the rules they used was that no sp^3 carbons could be adjacent—that is, the brominated carbons must form an independent set.

Fajtlowicz and Larson show that the independence number of a graph is a very good predictor of fullerene stability: more precisely, they show that the smallest stable fullerene isomers tend to minimize their independence numbers and that, for these stable isomers, minimization of independence number is a better predictor of stability than maximization of the HOMO-LUMO gap.[16]

3. Definitions & Examples

The *independence number* α of a graph is the cardinality of a maximum independent set. For example, in the graph in Fig. 1, $\alpha = 3$.

A set F is a *forcing set* for a maximum independent set I if $F \subseteq I$ and I is the only maximum independent set that contains F. By the definition, a forcing set F for a maximum independent set I is necessarily independent. The *forcing number* $f(I)$ of a maximum independent set I is the cardinality of a minimum forcing set

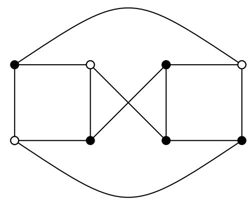

FIGURE 1. The set of white vertices is a maximum independent set.

for I. The *forcing number* $f(G)$ of a graph G is the minimum value of $f(I)$ for all maximum independent sets I. It may seem potentially confusing to use the same vocabulary and notation for two different concepts—in fact, which concept is meant will always be clear from the context.

Let P_n be the path on n vertices. See Fig. 2 for two examples. The graph P_3 on the left has $\alpha = 2$. The white vertices I are a maximum independent set. This is the unique maximum independent set for the graph. The forcing number $f(I)$ for I is 0. Thus the forcing number $f(P_3)$ for P_3 is 0. The graph P_4 on the right also has $\alpha = 2$. The white vertices J are a maximum independent set. $F = \{v_3\}$ is a minimum forcing set for J. The forcing number $f(J)$ for J is 1. No maximum independent set with a smaller forcing set can be found. Thus the forcing number $f(P_4)$ for P_4 is 1. It can further be argued, $f(P_n) = 0$ if n is odd and $f(P_n) = 1$ if n is even.

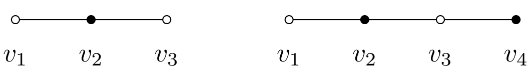

FIGURE 2. $f(P_3) = 0$ and $f(P_4) = 1$

The forcing number of different maximum independent sets in a graph can be different. See Fig. 3 for an example. This graph has independence number $\alpha = 3$. The sets of white vertices are maximum independent sets. The forcing number of the set of white vertices on the left is 2, while the forcing number of the set of white vertices on the right is 1.

Computations show that the values of the forcing number are relatively small for small connected graphs. This data is compiled in Table 3.

It is clear that, for any graph, $0 \leq f \leq \alpha$. Examples can be found which give equality in these bounds. The path P_3 on three vertices gives an example where

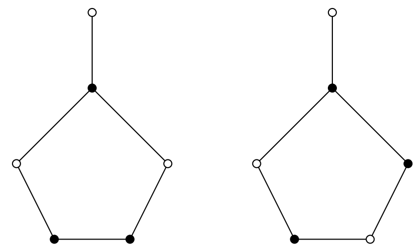

FIGURE 3. Forcing numbers for different maximum independent sets can be different: the indicated maximum independent sets have forcing numbers 1 and 2.

n	$f=0$	$f=1$	$f=2$	$f=3$	$f=4$
1	1				
2		1			
3	1	1			
4	2	4			
5	8	11	2		
6	35	68	9		
7	252	524	75	2	
8	2994	7161	934	28	
9	68665	171684	20296	432	3
10	3013075	7849829	840786	12766	115

TABLE 1. Forcing numbers for connected graphs of order n.

$f=0$. The flower F_4 in Fig. 3 is an example where $f=\alpha$. We will characterize the graphs for which equality holds in both the upper and lower bounds.

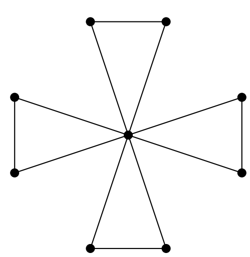

FIGURE 4. A flower F_4 with four petals. The forcing number is 4.

4. Fundamental Results

The independence number of a graph "behaves nicely": if you remove a vertex from the graph the independence number will not increase. Similarly, for any induced subgraph H of a graph G, $\alpha(H) \leq \alpha(G)$. The same is not true for the forcing number of a graph. The forcing number of a subgraph may be smaller or larger than the forcing number of the parent graph. For example, P_1 is a subgraph of P_2 and $f(P_1) \leq f(P_2)$; but P_2 is an induced subgraph of P_3 and $f(P_2) \geq f(P_3)$. Fortunately, the forcing number does have some useful properties.

Let G be a graph with vertex set $V(G)$. If a vertex v is adjacent to a vertex w we write $v \sim w$. The *(open) neighborhood* $N(v)$ of a vertex v is the set of vertices adjacent to v; that is $N(v) = \{w : v \sim w\}$. The *closed neighborhood* $N[v]$ of a vertex v is $N(v) \cup \{v\}$. These notions can be generalized to sets: the (open) neighborhood of a set S is $N(S) = \cup_{v \in S} N(v)$, and the closed neighborhood of a set S is $N[S] = N(S) \cup S$. If $S \subseteq V(G)$, the *induced subgraph* $G[S]$ is the graph with vertex set S and edge set $\{xy : x, y \in S \text{ and } x \sim y\}$, that is, there is an edge between two vertices of the induced subgraph if and only if there is an edge between the vertices in the parent graph G. For convenience, we use $G - S$ to denote the graph $G[V(G) \setminus S]$ induced on the remaining vertices after deleting the vertices in S.

The following result is a useful tool and, furthermore, provides some intuition of the role of forcing sets in the independence structure of a graph.

Proposition 4.1. *If F is a forcing set for a graph G then $G - N[F]$ has a unique maximum independent set.*

Proof. Let F be a forcing set of G corresponding to a maximum independent set I. So $I - F$ is a maximum independent set of $G - N[F]$. Suppose J is a maximum independent set of $G - N[F]$. So $F \cup J$ is a maximum independent set of G. Since F is a forcing set for G it follows that $F \cup J = I$ and $J = I - F$. That is, $G - N[F]$ has a unique maximum independent set. □

The following result shows that the forcing number of a graph is bounded by a function of the number of maximum independent sets of the graph.

Proposition 4.2. *Let M be the number of maximum independent sets in a graph. For any graph, $f \leq M - 1$.*

Proof. Let G be a graph and $I_1, I_2, \ldots, I_M$ be the maximum independent sets in G. For $i \in \{1, \ldots, M-1\}$, let $v_i \in I_M \setminus I_i$. Let $F = \{v_1, \ldots, v_{M-1}\}$. $F \subseteq I_M$, and

$F \not\subseteq I_i$, for $i \in \{1, \ldots, M-1\}$. So F is a forcing set for I_M. Thus $f = f(G) \leq f(I_M) \leq |F| \leq M - 1$. $\square$

A *support vertex* of a graph is a vertex adjacent to a pendant vertex. So the path P_3 has a single support vertex, and any longer path has two support vertices. Notice that a set consisting of a single support vertex is a minimum forcing set for any path P_{2n} with even order: the graph formed by deleting this set and its neighbors has a unique independent set.

The main idea of the following five propositions is that vertices which are in every maximum independent set or vertices which are not in any maximum independent set play a special role in the theory of minimum forcing sets. Any vertex which is in every maximum independent set will not be included in a minimum forcing set, and vertices which are not in any maximum independent set can be deleted: a set is a minimum forcing set for the reduced graph if and only if it is a minimum forcing set for the parent graph.

Proposition 4.3. *If v is in every maximum independent set of a graph G then $f(G) = f(G - N[v])$.*

Proof. Suppose v is in every maximum independent set of a graph G.

First we show that $f(G) \leq f(G - N[v])$. Let F be a minimum forcing set for $G - N[v]$ corresponding to a maximum independent set I of $G - N[v]$. So $|F| = f(G - N[v])$. Then $I' = I \cup \{v\}$ is a maximum independent set in G. Let J be a maximum independent set of G containing F. $J - v$ is a maximum independent set of $G - N[v]$. Since F is a forcing set for $G - v$ it follows that $J - v = I - v$. So $J = I$ and $f(G) \leq |F|$.

Now we show that $f(G - N[v]) \leq f(G)$. Let F be a minimum forcing set for G and I be a corresponding maximum independent set. So $v \in I$, $f(G) = |F|$, and $I - v$ is a maximum independent set in $G - N[v]$.

We will now show that $F - v$ is a forcing set for $I - v$ in $G - N[v]$. $F - v$ is an independent subset of the maximum independent set $I - v$. Suppose J is a maximum independent set of $G - N[v]$ containing $F - v$. So $J' = J \cup \{v\}$ is a maximum independent set of G containing F. Since F is a forcing set for I, it follows that $J' = I$, and $J = I - v$. So $f(G - N[v]) \leq |F - v| \leq |F| = f(G)$. $\square$

The *core* of a graph is the set of vertices belonging to all maximum independent sets; thus $core(G) = \cap\{I : I \text{ is a maximum independent set in } G\}$. Let $\xi(G) = |core(G)|$. The core of a graph is a fundamental concept in the theory of maximum independent sets of a graph. See Ref. 17 for more information and results. In Ref. 18 Hammer, Hansen and Simeone show that finding the core of a graph is

NP-complete. Let the *anti-core* of a graph be the set of vertices which are not in any maximum independent set. These are fundamental concept in the theory of forcing independent sets as minimum forcing independent sets cannot contain vertices from either the core or anti-core.

Proposition 4.4. *If G is a graph then $f \leq \alpha - \xi$.*

Proof. Let $core(G) = \{v_1, \ldots, v_\xi\}$ and let $I = \{v_1, \ldots, v_\xi, v_{\xi+1}, \ldots, v_\alpha\}$ be a maximum independent set. Let $F = \{v_{\xi+1}, \ldots, v_\alpha\}$. Since F is a forcing set for I, it follows that $f(G) \leq |F| = |I| - |core(G)| = \alpha - \xi$. □

Proposition 4.5. *For any graph G, $f(G) = f(G - N[core(G)])$.*

Proof. One proof can be constructed by directly imitating the proof of Proposition 4.3. Another proof can be constructed by repeated application of this proposition. Suppose $core(G) = \{v_1, v_2, \ldots, v_\xi\}$ is the set of vertices in every maximum independent set of G. Let $G = G_1$. So, $f(G) = f(G_1) = f(G_1 - N[v_1])$. It is easy to see that v_2 is in every maximum independent set of $G_2 = G_1 - N[v_1]$. Thus $f(G_2) = f(G_1 - N[v_1] - N[v_2]) = f(G_1 - N[\{v_1, v_2\}])$. So $f(G) = f(G_1) = f(G_2) = \ldots = f(G_{\xi+1})$. It then follows that $f(G) = f(G_{\xi+1}) = f(G - N[core(G)])$. □

Proposition 4.6. *If v is in the anti-core of a graph G then $f(G) = f(G - v)$.*

Proof. First note that if v is in the anti-core of G then $\alpha(G) = \alpha(G - v)$. Now let F be a minimum forcing set of G, corresponding to a maximum independent set I; so $f(G) = |F|$. So I is also a maximum independent set of $G - v$. It is easy to see that F is a forcing set for I in $G - v$. Thus $f(G - v) \leq |F| = f(G)$.

Now let F' be a minimum forcing set for $G - v$, corresponding to a maximum independent set I'. Since v is not in any maximum independent set, I' is also a maximum independent set in G. Suppose J is a maximum independent set of G with $F' \subseteq J$. Since J is a also a maximum independent set in $G - v$, and F' is a forcing set, it follows that $J = I'$ and F' is a forcing set in G. So $f(G) \leq |F'| = f(G - v)$. Thus $f(G) = f(G - v)$, which was to be shown. □

The main idea of the following proposition and its corollary is that the search for minimum forcing sets can be reduced to searching for minimum forcing sets in components of the graph. For graphs G, G_1, G_2, we write $G = G_1 \cup G_2$ if G is the disjoint union of G_1 and G_2.

Proposition 4.7. *If $G = G_1 \cup G_2$ then $f(G) = f(G_1) + f(G_2)$.*

Proof. Let F be a minimum forcing set for G corresponding to a maximum independent set I. Let $F_1 = F \cap V(G_1)$, $F_2 = F \cap V(G_2)$, $I_1 = I \cap V(G_1)$, and $I_2 = I \cap V(G_2)$.

First we will show that F_1 is a forcing set for G_1. Note that $F_1 \subseteq I_1$. Suppose J_1 is a maximum independent set of G_1 with $F_1 \subseteq J_1$. Then $F \subseteq J_1 \cup I_2$. Since F is a forcing set for G it follows that $I_1 \cup I_2 = J_1 \cup I_2$ and $I_1 = J_1$. Similarly it follows that F_2 is a forcing set for G_2. So $f(G_1)+f(G_2) \leq |F_1|+|F_2| = |F_1 \cup F_2| = |F| = f(G)$.

Now let F_1 be a minimum forcing set for G_1, corresponding to a maximum independent set I_1; and let F_2 be a minimum forcing set for G_2, corresponding to a maximum independent set I_2. $I = I_1 \cup I_2$ is a maximum independent set of G. We will show that $F_1 \cup F_2$ is a forcing set for G. Let J be a maximum independent set of G with $F_1 \cup F_2 \subseteq J$. Let $J_1 = J \cap V(G_1)$ and $J_2 = J \cap V(G_2)$. Since F_1 is a forcing set for I_1 and $F_1 \subseteq J_1$, it follows that $I_1 = J_1$. Similarly it follows that $I_2 = J_2$. Thus $I = J$ and $F_1 \cup F_2$ is a forcing set for G. So $f(G_1) + f(G_2) = |F_1| + |F_2| = |F_1 \cup F_2| \geq f(G)$. □

Corollary 4.8. *If G is a graph with components $G_1, \ldots, G_k$ then $f(G) = \sum_{i=1}^{k} f(G_i)$.*

5. Graphs where $f = 0, k, \alpha$

5.1. Unique Maximum Independent Sets and Graphs where $f = 0$.

The forcing number of a graph is no less than 0 and no more than the independence number of the graph. We now turn to characterizing graphs having specific forcing numbers.

Any path P_n with odd n is an example of a graph with a unique maximum independent set. If a graph G has a unique maximum independent set I then clearly the empty set is a forcing set for I and $f(G) = 0$. The converse is also true.

Proposition 5.1. *$f = 0$ if and only if G has a unique maximum independent set.*

Proof. Let G be a graph. Assume first that G has a unique maximum independent set I. The empty set $\emptyset \subseteq I$ is a forcing set for I. Suppose J is a maximum independent set containing $\emptyset$. Since I is a unique maximum independent set, we have $I = J$. So $f(I) = 0$, and $f(G) = 0$.

Assume then that $f(G) = 0$. Let F be a minimum forcing set in G corresponding to a maximum independent set I; so $f(I) = 0$ and $F = \emptyset$. Let J be any maximum independent set of G. Since $\emptyset$ is a forcing set for G, and $\emptyset \subseteq J$, it follows that $I = J$. Since any maximum independent set is identical to I, I is a unique maximum independent set. □

It now follows immediately that any odd path P_{2n+1} has forcing number $f = 0$.

5.2. Graphs where $f \leq k$.

Proposition 5.2. *For any non-negative integer k, $f \leq k$ if and only if there is an independent set F so that $G - N[F]$ has a unique maximum independent set of size at least $\alpha(G) - k$.*

Proof. Let G be a graph with $f \leq k$. Let $F = \{v_1, \ldots, v_f\}$ be a minimum forcing set for G corresponding to a maximum independent set $I = \{v_1, \ldots, v_f, v_{f+1}, \ldots, v_\alpha\}$. So $|F| = f \leq k$. Since F is a forcing set, Proposition 4.1 implies that the graph $G - N[F]$ has a unique maximum independent set. Since $\{v_{f+1}, \ldots, v_\alpha\}$ is an independent set in $G - N[F]$, it follows that $\alpha(G - N[F]) \geq \alpha(G) - f \geq \alpha(G) - k$, which was to be shown.

Assume now that there is an independent set F so that $G - N[F]$ has a unique maximum independent set F' of size at least $\alpha(G) - k$. Clearly $f \leq |F|$. Let $I = F \cup F'$. Then $\alpha \geq |I| = |F| + |F'| \geq f + (\alpha(G) - k)$. It follows that $f \leq k$. □

Notice that an even path does not have a unique maximum independent set. So $f(P_{2n}) \geq 1$. Note too that if you remove a support vertex of an even path, together with its neighbors, the remaining graph is an odd path with a unique maximum independent set. Since there is a maximum independent set containing this support vertex, it then follows that $f(P_{2n}) \leq 1$. So $f(P_{2n}) = 1$. A similar argument can be made to determine the forcing number of an even cycle. Here, $f(C_n) = 1$.

In the case of an odd cycle (with $n \geq 5$), note that the removal of a single vertex and its neighbors gives a non-trivial even path—which does not have a unique maximum independent set. So $f(C_{2n+1}) > 1$. If two vertices v and w which are connected by a path of length 3 (so this path has 4 vertices) and their neighbors are removed, an even path is removed, leaving an odd path with a unique maximum independent set. Proposition 5.2 then implies that $f \leq 2$. So, $f(C_{2n+1}) = 2$.

5.3. **Graphs where $f = \alpha$.** For every value of the independence number α, there are graphs where $f = \alpha$. One example is the class of *flowers* F_k. F_k is formed by identifying one vertex in each of k copies of the triangle K_3; the triangles become petals in the flower. (See Fig. 3 for an example of F_4.) In F_k the center vertex is not in any maximum independent set. Deletion of this vertex yields k copies of the edge K_2. Each maximum independent set of F_k contains exactly one vertex from each K_2. So we have that for the flowers, $f(F_k) = \alpha(F_k) = k$.

Proposition 5.3. *$f = \alpha$ if and only if there is no independent set J with $|J| = \alpha - 1$ and $|V - N[J]| = 1$.*

Proof. Assume first that $f = \alpha$. Suppose there is an independent set J with $|J| = \alpha - 1$ and $|V - N[J]| = 1$. So $V \setminus (J \cup N(J)) = \{v\}$, for some vertex

v. $G[\{v\}]$ has a unique maximum independent set. Thus Proposition 4.1 implies that J is a forcing set for the maximum independent set $I = J \cup \{v\}$. But then $f(G) \leq |J| = \alpha - 1$, contradicting the fact that $f = \alpha$.

Assume then that there is no independent set J with $|J| = \alpha - 1$ and $|V - N[J]| = 1$. Let $I = \{v_1, \ldots, v_\alpha\}$ be a maximum independent set for G. Let $J = \{v_1, \ldots, v_{\alpha-1}\}$. By assumption $G - N[J]$ has at least two vertices, one of which is v_α. So J is not a forcing set for I. Since this argument holds for any $v_i \in I$, $f(I) = \alpha$. And since this argument holds for any maximum independent set, $f(G) = \alpha$, which was to be shown. $\square$

Proposition 5.4. *If $f = \alpha$ then $n - |\text{anti-core}| \geq 2\alpha$.*

Proof. Let G be a graph. Let I be a maximum independent set of G. Assume that $f = \alpha$. So $\alpha = |I|$. For every $v \in I$ let $I_v = I - v$. Proposition 5.3 implies that $|V - N[I_v]| > 1$. The proof of Proposition 5.3 shows that there must be at least two vertices in $V - N[I_v]$ which are each in some maximum independent set (and thus not in the anti-core). Let v' be any vertex in $V - N[I_v]$ besides v which is not in the anti-core. Let $J = \{v' : v \in I\}$. The vertices in J are distinct from each other and distinct from the vertices in I, and none are in the anti-core of G. Thus the claim follows. $\square$

6. Benzenoids

Benzenoids are graphs which can be represented as a subgraph of the infinite hexagonal lattice formed by taking a closed curve along the edges of this lattice. See Ref. 19 for some basic facts about these graphs and their utility in representing molecules of the same name. They are bipartite. Recall that ν is the matching number of a graph and that $\alpha + \nu = n$ for bipartite graphs (the König-Egerváry Theorem). It follows that a non-trivial bipartite graph has at least two maximum independent sets and thus $f \geq 1$. See Fig. 5 for an example. Both the white and black sets of vertices are a maximum independent set. This benzenoid has a perfect matching. Any choice of a vertex in this graph uniquely picks out an associated maximum independent set. So $f = 1$. Note that having a perfect matching does not always imply that there are exactly 2 maximum independent sets. The benzenoid in Fig. 6 has a perfect matching 3 maximum independent sets. Whether having a perfect matching implies that $f = 1$ is an open question.

The class of triangulenes include examples of benzenoids with unique maximum independent sets and, thus, forcing number $f = 0$. See Fig. 7 for the first three triangulenes; T_1, T_2, and T_3. The white sets of vertices are maximum independent sets. It is easy to see that $f(T_1) = 1$. In T_2 at most half of the vertices in the

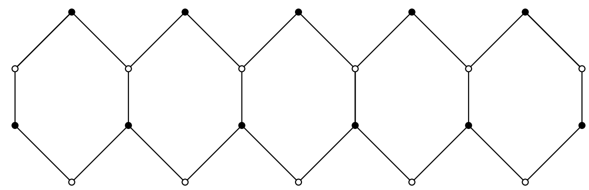

Figure 5. A linear benzenoid chain.

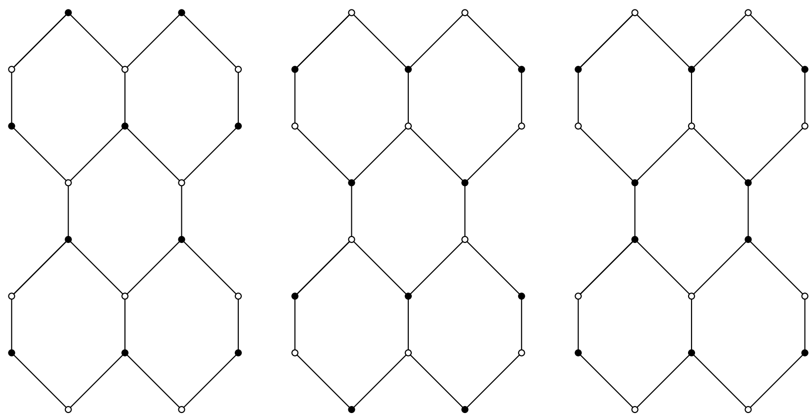

Figure 6. The three maximum independent sets in the smallest hourglass benzenoid.

outside cycle belong to a maximum independent set. Since the center vertex can be added to a choice of half of the vertices of the outside cycle, it follows that this is a maximum independent set. Since the outside cycle has exactly two maximum independent sets, T_2 has a unique maximum independent set. Thus, $f(T_2) = 0$. A similar argument shows that $f(T_3) = 0$.

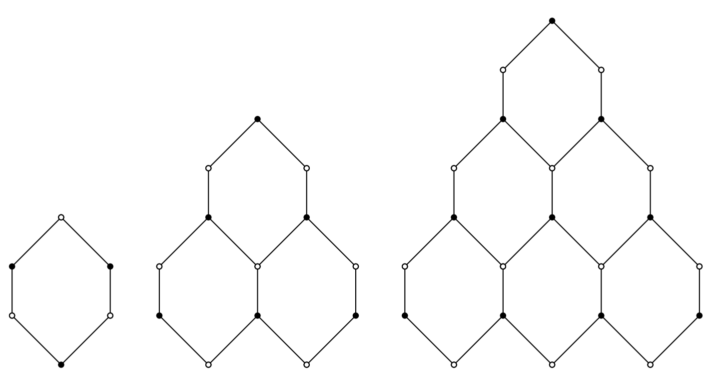

Figure 7. The first three triangulenes; T_1, T_2, and T_3. $f(T_1) = 1$, while $f(T_2) = f(T_3) = 0$.

For "small" benzenoids with no more than 12 hexagons the forcing number f is either 0 or 1. Calculations show that the situation becomes more interesting for benzenoids with more than 12 hexagons; see Table 6. The program *benzene* was used to generate complete lists of non-isomorphic benzenoids.[20] The forcing numbers were calculated using a straight-forward algorithm which checks all subsets of the maximum independent sets until a smallest forcing set is found. The program uses some bounding criteria and optimizations, but is still quite slow when the forcing number and the independence number are high. The program *Cliquer* was used to find all the maximum independent sets.[21]

hexagons	$f = 0$	$f = 1$	$f = 2$
1		1	
2		1	
3	1	2	
4	1	6	
5	7	15	
6	30	51	
7	141	190	
8	668	767	
9	3249	3256	
10	15666	14420	
11	75931	65298	
12	367664	301920	
13	1781841	1416398	17
14	8636667	6730574	336
15	41888162	32315128	4620

TABLE 2. Forcing number data for benzenoids with 1 to 15 hexagons.

7. Open Problems

(1) *Forcing Ratio.* The *forcing ratio* $\frac{f}{n}$ of a graph may be of some interest. Large paths representing molecular chains should be expected to have similar properties. But, as we saw, odd paths and even paths have different forcing numbers: 0 for odd paths and 1 for even paths. In both cases though the forcing ratio goes to 0. In this sense, long odd and even paths really are "the same". For flowers F_n the forcing ratio is $\frac{n}{2n+1}$, which goes to $\frac{1}{2}$ in the limit. Can a graph have a forcing ratio greater than $\frac{1}{2}$?

(2) *Well-Covered Graphs.* A graph is *well-covered* if every maximal independent set is a maximum independent set. The theory of well-covered graphs was initiated by Plummer[22] in 1970 and has been extensively pursued since then. The interest in well-covered graphs lies partly in the fact that these are graphs where any greedy algorithm for finding a maximal independent set yields a maximum independent set. Notice that for flowers F_k the center vertex is not in any maximum independent set. It is the only vertex with this property. Upon removing the center vertex, the remaining graph is well-covered. Note too that well-covered graphs necessarily have an empty anti-core.

Conjecture 7.1. *If G is a graph with an empty anti-core and $f = \alpha$ then G is well-covered.*

The converse is not true. The graph P_4 is a counterexample: P_4 is well-covered and has an empty anti-core, but $f = 1$ and $\alpha = 2$.

(3) *Benzenoids.* When looking at the benzenoids with $f = 2$, we see that most of them consist of a large part with a fixed maximum independent set (N[core]) and 2 smaller subgraphs which each have 2 maximum independent sets. This seems to suggest that any value for the forcing number of benzenoids is possible, as long as the benzenoids are sufficiently large.

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Department of Mathematics and Applied Mathematics, Virginia Commonwealth University, Richmond, VA 23284, phone: (804) 828-5576, fax: (804) 828-8785

E-mail address: clarson@vcu.edu

Department of Applied Mathematics, Computer Science & Statistics, Ghent University, 9000 Ghent, Belgium

E-mail address: nico.vancleemput@gmail.com