HKD 1926 CROATICA CHEMICA ACTA

CROATICA CHEMICA ACTA
CCACAA, ISSN 0011-1643, e-ISSN 1334-417X
Croat. Chem. Acta **86** (4) (2013) 469–475.
http://dx.doi.org/10.5562/cca2295

Original Scientific Article

Forcing Independence[†]

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RECEIVED MAY 23, 2013; REVISED OCTOBER 18, 2013; ACCEPTED OCTOBER 21, 2013

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. (doi: 10.5562/cca2295)

Keywords: forcing, independent set, independence number, benzenoids

1. DEDICATION

The authors dedicate this article to Prof. Douglas Klein on occasion of his 70th 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 of no more than one vertex of "small" benzenoids identifies the unique maximum independent set containing that vertex (see Figures 4. and 6.).

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 existing concepts defined for matchings, discussed in the next section. 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. The *matching number* is the cardinality of a maximum matching. If the edges of a matching 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

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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 Živković 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 number (of a maximum matching) 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 *independence number* α of a graph is the cardinality of a maximum independent set of vertices. Let n be the number of vertices (or *order*) of a graph. Then 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 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.[13] Merrifield and Simmons show that the number σ of independent sets of vertices 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. The paper of Fajtlowicz and Larson[16] suggests a connection between fullerene stability and independence number minimization; Fowler, Daugherty and Myrvold[17] argue that there are better chemical explanations for the observed correlation.

3. DEFINITIONS & EXAMPLES

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 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 Figure 1. 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.

The forcing number of different maximum independent sets in a graph can be different. See Figure 2. 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.

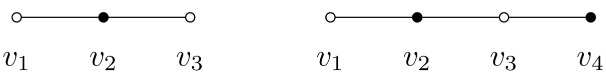

Figure 1. $f(P_3) = 0$ and $f(P_4) = 1$.

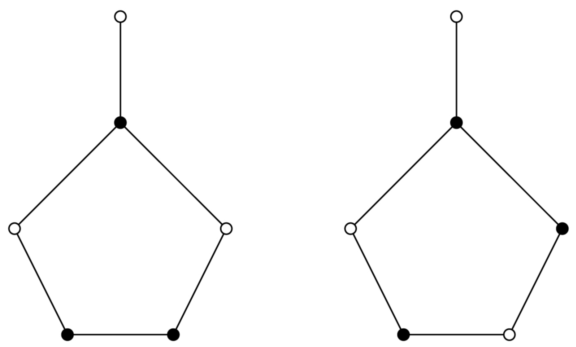

Figure 2. Forcing numbers for different maximum independent sets in a graph can be different. The forcing number for the indicated maximum independent set (the white vertices) in the left graph is 2, while the forcing number for the indicated maximum independent set in the right graph is 1.

Table 1. The distribution of forcing numbers for all connected graphs of order no more than 10

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

Computations show that the values of the forcing number are relatively small for small connected graphs. This data is compiled in Table 1.

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

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. In the case where $S = \{v\}$, we write $G - v$.

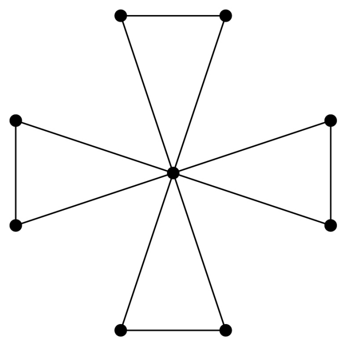

Figure 3. A flower F_4 with four petals. The forcing number is 4.

One referee has pointed out that the concepts of a forcing set and a jet set are related. A *jet* is a set of vertices where the complement of its neighborhood is a maximum independent set.[18,19] So, for instance, in P_3, the set S consisting of a single pendant vertex is a jet of P_3–as its neighborhood $N(S)$ is the set containing the middle vertex, and the complement of $N(S)$ is the set of both pendant vertices, which is a maximum independent set. Note that S is also a forcing set for this maximum independent set.

It is not difficult to show that every jet set is a forcing set. In general, forcing sets for maximum independent sets are not jet sets. In P_3 the empty set is a (minimum) forcing set for the unique maximum independent set, while the empty set is not a jet set. In P_6 the (unique) neighbor of either of the pendant vertices is a (minimum) forcing set for the unique maximum independent set containing that vertex–but it is not a jet set.

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.

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 $M(G)$ be the number of maximum independent sets in a graph G. For any graph G, $f(G) \leq M(G) - 1$.*

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 $F \nsubseteq I_i$, for $i \in \{1, \ldots, M-1\}$. So F is a forcing set for I_M. Thus $f(G) \leq f(I_M) \leq |F| \leq M - 1$. □

A support vertex of a graph is a vertex adjacent to a pendant vertex. So the path P_3 has one 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 $G - N[v]$ 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 $f(G - N[v]) \leq |F - v| \leq |F| = f(G)$. □

The core of a graph is the set of vertices belonging to all maximum independent sets; thus $core(G) = \cap\{I : I$ 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. 20 for more information and results. In Ref. 21 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 concepts 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 $f(G) \leq \alpha(G) - \xi(G)$.*

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 $f(G) \leq |F| = |I| - |core(G)| = \alpha(G) - \xi(G)$. □

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 $f(G) = f(G_1) + f(G_2)$.*
Corollary 4.8. *If G is a graph with components $G_1, \dots, G_k$ 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. *$f(G) = 0$ if and only if G has a unique maximum independent set.*

It 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 graph G and non-negative integer k, $f(G) \leq k$ 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 $F = \{v_1, \dots, v_f\}$ be a minimum forcing set for G corresponding to a maximum independent set $I = \{v_1, \dots, v_f, v_{f+1}, \dots, v_\alpha\}$. 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 $\{v_{f+1}, \dots, v_\alpha\}$ 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 Figure 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. *For any graph G, $f(G) = \alpha(G)$ if and only if there is no independent set J with $|J| = \alpha(G) - 1$ and $|V - N[J]| = 1$.*
Proof. Let G be a graph. Assume first that $f(G) = \alpha(G)$. 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 $f(G) \leq |J| = \alpha(G) - 1$, contradicting the fact that $f(G) = \alpha(G)$.
Assume then that there is no independent set J with $|J| = \alpha(G) - 1$ and $|V - N[J]| = 1$. Let $I = \{v_1, \dots, v_\alpha\}$ be a maximum independent set for G. Let $J = \{v_1, \dots, v_{\alpha-1}\}$. 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 $v_i \in I$, $f(I) = \alpha(G)$. And since this argument holds for any maximum independent set, $f(G) = \alpha(G)$, which was to be shown. □
Proposition 5.4. *For any graph G, if $f(G) = \alpha$ then $n(G) - |\text{anti-core}| \geq 2\alpha(G)$.*
Proof. Let G be a graph. Let I be a maximum independent set of G. Assume that $f(G) = \alpha(G)$. 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. □

6. BENZENOIDS

Benzenoids are graphs which can be represented as a subgraph of the infinite hexagonal lattice formed by

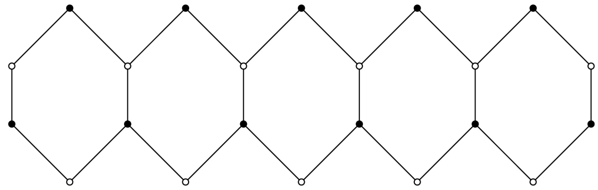

Figure 4. A linear benzenoid chain.

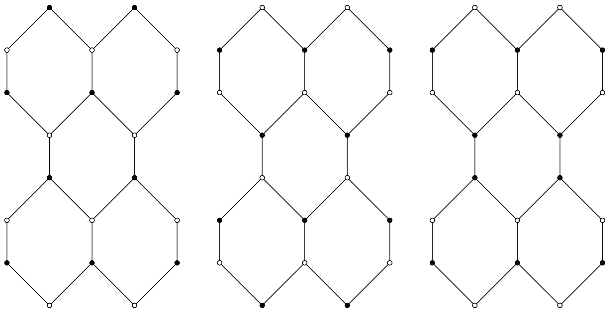

Figure 5. The three maximum independent sets in the smallest hourglass benzenoid.

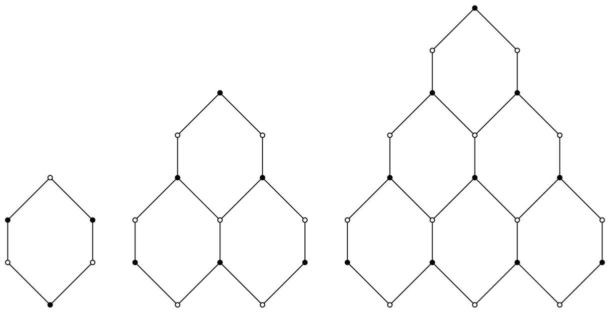

Figure 6. The first three triangulenes; T_1; T_2, and T_3. $f(T_1) = 1$, while $f(T_2) = f(T_3) = 0$.

taking a closed curve along the edges of this lattice. See Ref. 22 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 bipartite graph (with at least two vertices) has at least two maximum independent sets and thus $f \geq 1$. See Figure 4. 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 Figure 5. has a perfect matching and 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 Figure 6. 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 outer cycle belong to a maximum independent set. Since there is an independent set containing half of these vertices together with the remaining (center) vertex, it is a maximum independent set. And since there is a unique independent set in the outer cycle that can be added to the center vertex to form a maximum independent set, it follows that T_2 has a unique maximum independent set and $f(T_2) = 0$. A similar argument shows that $f(T_3) = 0$.

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 2. The program *benzene* was used to generate complete lists of non-isomorphic benzenoids.[23] 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.[24]

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 *maximal* independent set is an independent set which is not a subset of any larger independent set. Maximal independent sets may be, but are not necessarily, maximum. For instance, let S be the set consisting of the center vertex of P_3. S is a maximal independent set which is not a maximum independent set.

A graph is *well-covered* if every maximal independent set is a maximum independent set. The theory of well-covered graphs was initiated by

Table 2. The distribution of forcing numbers for all benzenoids with no more than 15 hexagonal faces

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

Plummer[25] 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 $f(G) = \alpha(G)$ 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.

Acknowledgements. The authors would like to thank the editor and referees for many useful suggestions that improved the clarity of the presentation. The first author would like to thank Prof D. J. Klein and the Welch Foundation of Houston, Texas, for support for this research, under grant BD-0894.

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