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CUT–EDGES AND THE INDEPENDENCE NUMBER

Ryan Pepper [a,1], Greg Henry [b], Dillon Sexton [b]

[a] *Department of Computer and Mathematical Sciences, University of Houston – Downtown, Houston, TX 77002, USA*
(Second Address of First Author)
Texas A & M University at Galveston, Galveston, TX 77553, USA

[b] *Department of Mathematics, University of Houston, Houston, TX 77204,USA*

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ABSTRACT: The graph theoretic independence number has recently been linked to fullerene stability [2, 4]. In particular, Fajtlowicz formed the hypothesis – based on conjectures of the program Graffiti – that stable fullerenes tend to minimize their independence numbers. More recently, it was noticed that stable benzenoids do minimize their independence numbers [3, 5, 7, 8]. In this paper, we prove a lower bound on the independence number as a function of the number of cut-edges in the graph. Equality holds for this lower bound only for trees with perfect matchings, from which, since chemical trees with perfect matchings are generally more stable than those without, we infer that stable acyclic conjugated hydrocarbons also minimize their independence numbers – analogous to their benzenoid and also perhaps to their fullerene cousins. Together, this evidence suggests that this simple graph invariant may play some significant role in organic chemistry.

[1] Corresponding Author

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1. Introduction

An **independent set** in a graph is a set of vertices with the property that no two vertices in the set are adjacent. The **independence number** of a graph G, denoted $\alpha(G)$ or simply α, is the cardinality of a largest independent set. This simple invariant is well studied in the graph theory literature, and to a lesser extent in chemistry. Having said this, it must be pointed out that for bipartite graphs – sometimes called alternate graphs – the independence number is intimately related to the matching number, which is the size of a largest collection of mutually non-incident edges (such a collection is called a matching) and which has been well studied in chemical graph theory. In particular, due to some early results in graph theory by Konïg (1931) and Gallai (1959), the sum of the independence number and the matching number of every bipartite graph is the number of vertices, or order, of the graph. When the matching number of a graph is half of its order, namely $\frac{n}{2}$, the matching is called perfect and is better known as a Kekulé structure in chemistry.

Recently, Fajtlowicz formed the hypothesis that stable fullerenes tend to minimize their independence numbers [2, 4]. This idea was inspired by conjectures of his computer program Graffiti. Some evidence for this hypothesis is that the stable forms of C_{60}, C_{70}, and C_{76} all uniquely minimize their independence numbers out of the many thousands of fullerene isomers in the respective classes [2].

In addition to this, it was noticed that stable benzenoids, close relatives of fullerenes, do indeed minimize their independence numbers [3, 5, 7, 8], lending some non-statistical evidence to the hypothesis. This is because stable benzenoids are bipartite graphs with perfect matchings, which implies that their independence numbers are $\frac{n}{2}$ by the previously mentioned corollary to Konïgs' and Gallais' theorems. However, $\frac{n}{2}$ is also a lower bound on the independence number for every bipartite graph, whence the independence number of stable benzenoids achieves its lower bound and in this sense, is minimized.

Here in this note, we present a lower bound on the independence number for all graphs and characterize the case of equality. Since it turns out that equality holds for and only for trees with perfect matchings – Kekulé structures – and since, in general, more stable acyclic hydrocarbons can be represented by such trees, we have yet more evidence for the independence-stability hypothesis for fullerenes.

2. Lower Bound

Definition 1. Let G be a graph (all graphs in this paper are simple and finite). A **cut-edge** of G, also called a bridge, is an edge whose deletion increases the number of components. If G is connected, then the deletion of a cut-edge leaves precisely two components. The total number of cut-edges in G will be denoted by $b(G)$ or simply b.

The program Graffiti made the following conjecture about cut-edges and the independence number during classroom use.

(1) $$\alpha(G) \geq \frac{b(G) + Q(G)}{2},$$

where $Q(G)$ is the number of odd components of G – an odd component refers to a component with an odd number of vertices.

Graffiti's conjecture 1 follows from a corollary to the theorem we prove in this note. Namely, we prove the following.

Theorem 1. *For every graph G,*

$$\alpha \geq \frac{b+1}{2}.$$

Corollary 2. *For every graph with $k \geq 1$ components,*

$$\alpha \geq \frac{b+k}{2}.$$

Graffiti's conjecture now follows from this corollary. A few more ideas are necessary before presenting a proof of Theorem 1.

A natural way to partition disconnected graphs is by their connected components. Should a graph be connected, we perform an analogous partitioning by considering as parts those vertex sets for which every pair of vertices in the set is joined by a path containing no cut-edges. To be more precise, we call a graph **cut-edge-connected** if every pair of vertices can be joined by a path containing no cut-edges. Let us call a maximal cut-edge-connected subgraph of a graph a **cut-edge-block**[2]. Now, with this notation in place, we will partition a connected graph so that each part is a cut-edge-block. Moreover, such a partitioning is unique and if H is a cut-edge-block, then any subgraph properly containing H will not be cut-edge-connected (since H is maximal).

[2]For discussion of similar structures involving cut-vertices rather than cut-edges, see [6].

Now, any edge joining vertices from distinct cut-edge-blocks must be a cut-edge. Form a graph whose vertex set is the set all cut-edge-blocks and whose edge set is the set of all cut-edges. This graph is clearly a tree since its edges are all cut-edges (which belong to no cycles). Two vertices in this tree are adjacent if and only if there is a pair of vertices x and y from the respective cut-edge-blocks which are adjacent. We refer to this structure as the **cut-edge-block-tree** of a given connected graph G. Now we can proceed with the proof of Theorem 1.

Proof. (Theorem 1) Let G' be the cut-edge-block tree of G. Let α' and n' be the independence number and order of G'. Since trees are bipartite, each part of a bipartite graph is an independent set, and at least one of the parts has at least half of the vertices, we know that $\alpha' \geq \frac{n'}{2}$. Also, $n' = b + 1$ since trees have one more vertex than edge and the edges of G' are precisely the b cut-edges of G. Now, every independent set $I \subseteq G'$ can be extended to an independent set of G with the same cardinality simply by taking one vertex in G from each of the cut-edge-blocks comprising the vertices of I. Together this yields the desired inequality and proves Theorem 1;

$$\alpha \geq \alpha' \geq \frac{n'}{2} = \frac{b+1}{2}. \tag{2}$$

□

Theorem 3. *G is a tree with a perfect matching if and only if*

$$\alpha = \frac{b+1}{2}.$$

Proof. Suppose G is a tree with a perfect matching. Then, via Konïg's theorem mentioned in the introduction, $\alpha = \frac{n}{2}$. Furthermore, since all of the edges are cut-edges in this case, $b = n - 1$ completing the implication.

Conversely, suppose that $\alpha = \frac{b+1}{2}$. Form the cut-edge-block tree G'. Since in this case equality must hold throughout Inequality 2, we find that $\alpha = \alpha' = \frac{n'}{2}$, whence G' must be a tree with a perfect matching. Now, if $G = G'$ then we are done, so we may assume without loss of generality that they are different. If G' is a path, there must be a vertex $v \in G'$ whose cut-edge-block in G has at least three vertices, say x, y, and z, such that at least one of these vertices is not part of a cut-edge. Without loss of generality, let x be the vertex in the cut-edge-block v not belonging to a cut-edge. Choose one vertex from each cut-edge-block of the part of G' not containing v, together with the vertex x, and we have formed an independent set in G with more than $\frac{n'}{2}$ vertices, a contradiction. Thus, we may assume that G' is not a path.

Let v be a branch point of G'. Let $A_1, A_2, \ldots, A_k$ be the branches stemming from v. Moreover, let $v_1, v_2, \ldots, v_k$ be the neighbors of v where v_i is the neighbor of v in A_i. Let M be the (unique) perfect matching of G' where, without loss of generality, v_1 is matched to v. Now form a set I by choosing the part of A_1 containing v_1 and for every $1 < i \leq k$, the part of A_i not containing v_i. This set has $\frac{n'}{2}$ vertices. Since the cut-edge-block v represents has at least three vertices and every edge emanating from it is a cut-edge in G, there is at least one vertex from this cut-edge-block which is not adjacent to v_1. Let x be such a vertex. The set $I \cup \{x\}$ is an independent set with more than $\frac{n'}{2}$ vertices, a contradiction. From this we must conclude that $G = G'$ – hence G is a tree with a perfect matching. $\square$

The proof of Graffiti's original conjecture given in Inequality 1 now follows from Corollary 2. The Corollary itself is quite evident since the independence number of a graph is the sum of the independence numbers of its components and the number of cut-edges of a graph is the sum of the number of cut-edges of its components.

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