Connected Graphs with Maximum Total Domination Number

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ABSTRACT. The total domination number $\gamma_t(G)$ of graph $G = (V, E)$ is the cardinality of a smallest subset S of V such that every vertex of V has a neighbor in S. It is known that, if G is a connected graph with n vertices, $\gamma_t(G) \leq \lfloor 2n/3 \rfloor$. Graphs achieving this bound are characterized.

1 Introduction

Let $G = (V, E)$ be a graph without loops or multiple edges and $n = |V|$. The familiar graphical invariant *domination number*, $\gamma(G)$, of G is the size of a smallest subset S of V such that every vertex of $V - S$ is adjacent to at least one vertex of S. While the domination number can be as large as n for the empty graph, Ore [3] has shown that $\gamma \leq \lfloor n/2 \rfloor$ when the graph has no isolated vertices. In particular, this bound is valid when the graph is connected and has at least two vertices. Payan and Xuong [4] characterized graphs with an even number of vertices which achieve the upper bound, and Cockayne, Haynes, and Hedetniemi [2] did the same when n is odd.

This paper is concerned with similar characterizations for the *total domination number*, $\gamma_t(G)$, defined as the size of a smallest subset S of V such that *every* vertex of V has a neighbor in S. Again an upper bound is available, this one provided by Cockayne, Dawes, and Hedetniemi [1].

Theorem 1 ([1]) *If G is a connected graph with $n \geq 3$ vertices, then $\gamma_t \leq \lfloor 2n/3 \rfloor$.*

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The need for a characterization of graphs achieving this upper bound arose from other studies being conducted by the authors related to certain allowable sequences of integers associated with the total domination number. Graphs achieving the bound are called *extremal*. It will be assumed in all discussions that the graphs of interest are connected.

Some notation is necessary. If X is a subset of V, then $N(X)$ ($N[X]$) is the open (closed) neighborhood of X and $\langle X \rangle$ is the subgraph of G induced by X. We say vertex u in set S has a *private neighbor* if $P_u = (V - S) \cap (N(u) - N[S - \{u\}]) \neq \emptyset$. The *private neighbors* of u are the vertices in P_u. Throughout this paper there will be many instances of the need for a phrase such as "the set $(S - \{a, b, c\}) \cup \{d, e\}$ obtained by removing vertices a, b, and c from S and including vertices d and e not in S is a smaller total dominating set, contradicting the assumption that S is a minimum total dominating set." For efficiency we will employ the following notation to represent this entire phrase: $\downarrow (a, b, c : d, e)$.

2 Preliminaries

The characterizations of those graphs G such that $\gamma_t(G) = \lfloor 2n/3 \rfloor$ of necessity requires examination of several cases. Some of the arguments are repetitive and this section presents lemmas useful in two or more of the cases.

The basis of all arguments is the structure of a minimum total dominating set S, as described in the proof of Theorem 1, and consequences of that structure. We review the pertinent points here and simultaneously take the opportunity to introduce some notation. Such an S can be partitioned as $A \cup B \cup C \cup D$ where

1. $A \cup B = \{v \in S : v$ has a private neighbor$\}$. We shall represent vertices of A by a_i for appropriate values of the index i, vertices of B by b_i, one private neighbor of a_i by w_i, and one private neighbor of b_i by v_i.

2. $B = \{v \in A \cup B : v$ is isolated in $\langle A \cup B \rangle\}$.

3. $C \subseteq S - (A \cup B)$ is a minimum size set such that each vertex of B is adjacent to some vertex of C. Usually, an element of C adjacent to b_i will be denoted c_i.

4. $D = S - (A \cup B \cup C)$.

Additional notation is included with the following facts shown in the proof of the theorem.

1. $|C| \leq |B|$.

2. $\langle D \rangle = mK_2$ for some nonnegative integer m. The vertices of the i^{th} K_2 are denoted by d_{i1} and d_{i2}.

3. For each i, at least one of d_{i1} and d_{i2}, say d_{i1} without loss of generality, is adjacent to a vertex $x_i \in V - S$.

4. x_i is adjacent to a second vertex of S.

5. d_{i1} and d_{i2} are not adjacent to x_j, $j \neq i$.

6. d_{i1} and d_{i2} are not adjacent to any vertex of $S - \{d_{i1}, d_{i2}\}$.

7. The bound of the theorem is established by the following sequence of equalities and inequalities:

$$|S| = \gamma_t(G) = (|A|+|B|+m)+(|C|+m) \leq 2(|A|+|B|+m) \leq 2(n-\gamma_t(G)).$$

In many cases of importance, it is possible to assume that $|D| = 0$, a fact derived in the following lemma. In the proof to this lemma we argue in detail the first two justifications showing that a particular configuration is impossible because it would produce a smaller total dominating set. In other cases, however, such detail will be omitted. It is helpful to keep in mind (1) that any a_i, b_i, c_i, d_{i1}, or d_{i2} is a member of S, and (2) vertices v_i, b_i, and c_i usually appear in this order as a path P_3 on three vertices.

Lemma 2 *If $n \geq 4$, $|A| = 0$, and $|V - S| = |B| + m$, then D may be taken to be empty.*

Proof: Since the v_i vertices are private neighbors, they are distinct from the x_i vertices. There must be at least $|B|$ vertices of type v_i and m of type x_i. This means that the $|B| + m$ vertices of $V - S$ have to be apportioned uniquely as private neighbors v_i for each $b_i \in B$ and neighbors x_i for each $d_{i1} \in D$. By facts 5 and 6 above and the private neighborness of the v_i, vertices d_{i1} and d_{i2} can be adjacent only to each other and to x_i. Thus the degree of d_{i1} is two. If the degree of d_{i2} is one, $\hat{S} = (S - \{d_{i2}\}) \cup \{x_i\}$ is another minimum total dominating set. Since d_{i1} is independent of every vertex of B, we see that, in $\hat{S}$, we may place d_{i1} in B and x_i in C, thereby eliminating d_{i1} and d_{i2} from D. The only remaining possibility is that the degree of d_{i2} is two so d_{i1}, d_{i2}, and x_i induce a triangle. Since $n \geq 4$, x_i must be adjacent to another vertex z. If $z \in S$, then, since x_i is adjacent to d_{i1}, d_{i2}, and z, we can produce a smaller total dominating set by replacing d_{i1} and d_{i2} with x_i, that is, $\downarrow (d_{i1}, d_{i2} : x_i)$. If z is not in S, then either $z = v_j$ or $z = x_j$ by the partitioning of $V - S$. Suppose $z = v_j$ so that we have the 3-path (v_j, b_j, c_j). If c_j has degree one in $\langle B \cup \{c_j\} \rangle$, then $\downarrow (c_j, d_{i1}, d_{i2} : v_j, x_i)$, that is, the subgraph induced by d_{i1}, d_{i2}, x_i, v_j,

b_j, and c_j is dominated by the three vertices x_i, v_j, and b_j instead of the original four vertices d_{i1}, d_{i2}, b_j, and c_j. If $z = v_j$ and c_j has degree at least two in $\langle B \cup \{c_j\}\rangle$, $\downarrow (b_j, d_{i1}, d_{i2} : v_j, x_i)$. Finally, if $z = x_j$, $j \neq i$, $\downarrow (d_{i1}, d_{i2}, d_{j1}, d_{j2} : x_i, x_j)$. Thus the degree of d_{i2} cannot be two and the result follows. □

The next result is key to determining allowable substructures of the extremal graphs.

Lemma 3 *Suppose b_i has a unique private neighbor v_i and $c_j \neq c_i$. If $C \cap N(b_k) \neq \{c_j\}$ for all $k \neq i, j$, then there is no path in G of the form (z, c_i, b_i, v_i, v_j) where $z \in S - \{c_j\}$.*

Proof: The condition on $N(b_k)$ indicates c_j is not necessary to dominate b_k. Therefore, if (v_j, v_i, b_i, c_i, z) is a path with $z \in S - \{c_j\}$, then $\downarrow (c_j, b_i : v_j)$. □

Lemma 3 leads to two useful corollaries. The first limits adjacencies between the v_i's.

Corollary 4 *If c_i is adjacent to $b_{i_1}, b_{i_2}, \ldots, b_{i_t}$ with $t \geq 2$, v_j is the unique private neighbor of b_{i_j}, and, for $k \neq i$, c_k has degree one in $\langle c_k \cup (B - \{b_{i_1}, b_{i_2}, \ldots, b_{i_t}\})\rangle$, then $v_j v_k \notin E$ for $1 \leq j \leq t$.*

The second corollary is a fundamental structural result. Define a *brush* to be a graph constructed from a connected graph M by identifying with each vertex of M one of the end vertices of a P_3. A brush is *nontrivial* if it is not a P_3, and the vertices of M form the *handle* of the brush. Note that a brush is also called the *2-corona* of a connected graph.

Corollary 5 *Let H be a subgraph induced by the $3t$ vertices of t paths of the form (c_i, b_i, v_i) where, in G, each b_i has degree two and $N(c_i) \cap B = b_i$. Then every component of H is either a C_6 or a brush whose handle, without loss of generality, is composed entirely of vertices of the type c_i.*

Proof: By hypothesis there are no edges of the form $c_i b_j$, $j \neq i$, and there can be none of the form $c_i v_j$ (here j may equal i) or $b_i v_j$, $j \neq i$, since v_i is a private neighbor of b_i. In other words, the only edges in H outside of those in the t paths are of the type $c_i c_j$ or $v_i v_j$. Suppose $v_i v_j$ and $c_i c_j$ are both edges so that $(c_i, b_i, v_i, v_j, b_j, c_j, c_i)$ forms a C_6. If v_i is adjacent to v_k, $k \neq j$, then $(c_j, c_i, b_i, v_i, v_k)$ is a path of the type forbidden by Lemma 3. By similar arguments there are no edges joining any of c_i, c_j, v_i, or v_j to any other vertices in H. Hence, the C_6 forms a component of H. By Lemma 3, if $c_i c_j$ is an edge and $v_i v_j$ is not, neither v_i nor v_j can have edges to any v_k, $k \neq i, j$, and the component is a brush whose handle is composed entirely of vertices of the type c_i. On the other hand, if $v_i v_j$ is an edge and $c_i c_j$

is not, Lemma 3 also implies there can be no edges from either c_i or c_j to any c_k, $k \neq i, j$. Thus the component containing edge $v_i v_j$ must be a brush whose handle is composed entirely of vertices of the type v_i. In this case we may create a new dominating set $\hat{S}$ by interchanging the labels v_i and c_i in the brush, where the new v_i (the old c_i) is now the private neighbor of b_i. We show $\hat{S}$ is a total dominating set. If this is not the case, then one of the original c_i was necessary to dominate another vertex $z \neq b_i$ in S. By the hypothesis $N(c_i) \cap B = b_i$, so $z \notin B$. Furthermore, every vertex of $A \cup C \cup D$ has a neighbor in S other than c_i, so no $z \in S$, other than b_i, depends on c_i for domination. Finally, $\hat{S}$ is minimum since it has the same cardinality as S. □

The next lemma is useful when a c_i is adjacent to two or more b_i's because it limits the number of edges which can be adjacent to the b_i's.

Lemma 6 *If c_i is adjacent to $b_{i_1}, b_{i_2}, \ldots, b_{i_t}$, at least one b_{i_j} is adjacent to no vertex of $S - \{c_i\}$.*

Proof: If, for each j, b_{i_j} is adjacent to $z_j \in S - \{c_i\}$, where the z_j need not be distinct, $S - \{c_i\}$ is a smaller total dominating set. □

3 The Cases

For an extremal graph, $\gamma_t(G) = \lfloor 2n/3 \rfloor$; hence, from fact 7,

$$\begin{aligned}\lfloor 2n/3 \rfloor &= |A| + |B| + |C| + 2m \leq 2(|A| + |B| + m) \leq 2(n - \lfloor 2n/3 \rfloor) \\ &= 2\lceil n/3 \rceil. \end{aligned} \tag{1}$$

We employ this to determine the various cases which must be considered, in the order in which it is convenient to do so.

Case 1. $n = 3k$. Then $\gamma_t = 2k = \lfloor 2n/3 \rfloor = 2\lceil n/3 \rceil$. Hence, the inequalities in Equation 1 are all equalities and $|A| + |B| = |C| \leq |B|$ by fact 1. It follows that $|A| = 0$, $|B| = |C|$, and $|S| = 2|B| + 2m$ implying $|V - S| = |B| + m$.

Case 2. $n = 3k + 2$. We have $\gamma_t = 2k + 1 = \lfloor 2n/3 \rfloor$ and $2\lceil n/3 \rceil = 2k + 2$. Thus $|C| \leq |A| + |B| \leq |C| + 1 \leq |B| + 1$, implying $|A| \leq 1$. By the definition of A, $\langle A \rangle$ has no isolated vertices so $|A| = 1$ is not possible and we conclude $|A| = 0$. This in turn implies $|C| \leq |B| \leq |C| + 1$. If $|B| = |C|$, $\gamma_t = 2|B| + 2m$ which is an even number, contradicting $\gamma_t = 2k + 1$. We are forced to conclude $|B| = |C| + 1$ implying $|S| = 2|B| - 1 + 2m = 2(|B| + m - 1) + 1$ and $|V - S| = |B| + m - 1 + 1 = |B| + m$.

Case 3. $n = 3k + 1$. Now $\gamma_t = 2k = \lfloor 2n/3 \rfloor$ and $2\lceil n/3 \rceil = 2k + 2$. Thus $|C| \leq |A| + |B| \leq |C| + 2 \leq |B| + 2$, implying $|A| \leq 2$. As before, $|A| \neq 1$. There are three subcases, two when $|A| = 0$ and one when $|A| = 2$. If $|A| = 0$, $|C| \leq |B| \leq |C| + 2$. If $|B| = |C| + 1$, $\gamma_t = 2|B| - 1 + 2m$ which is incorrectly odd. Thus, when $|A| = 0$, $|B| = |C|$ or $|B| = |C| + 2$.

Case 3a. $|A| = 0$, $|B| = |C|$, and $|S| = 2|B| + 2m$ implying $|V - S| = |B| + m + 1$.

Case 3b. $|A| = 0$, $|B| = |C| + 2$, and $|S| = 2|B| - 2 + 2m$ so $|V - S| = |B| - 1 + m + 1 = |B| + m$.

Case 3c. $|A| = 2$, $|B| = |C|$, and $|S| = 2|B| + 2 + 2m$ implying $|V - S| = |B| + 1 + m + 1 = |B| + m + 2$.

4 The Characterization When $n = 3k$

In this case we have $|A| = 0$, $|B| = |C|$, and $|V - S| = |B| + m$. The only connected graphs on three vertices are P_3 (which is a brush) and C_3, and they both have total domination number two. For other extremal graphs we may suppose $n \geq 6$ so we can use Lemma 2 to assume $|D| = 0$. It follows that $m = 0$ and $|V - S| = |B|$. Hence, letting P_B be the set of private neighbors of vertices in B, $V - S = P_B$ and $V = C \cup B \cup P_B$. By Lemma 6, there are no edges from c_i to $B - \{b_i\}$ for any i. Furthermore, there are no edges from v_i to $C \cup B - \{b_i\}$ since v_i is a private neighbor of b_i. Finally, the independence of B in $\langle A \cup B \rangle$ guarantees that none of the vertices in B are adjacent to each other. It follows that the only edges in G that are not of the type $c_i b_i$ or $v_i b_i$ are those between vertices in C or between vertices in P_B. This means each b_i has degree two and the entire graph G satisfies the conditions required for H in Corollary 5, so every component of G is either C_6 or a brush. Since G is connected, there is only one component and the characterization follows, with sufficiency an easy check.

Theorem 7 *A connected graph G with $n = 3k$ vertices has $\gamma_t = \lfloor 2n/3 \rfloor$ if and only if G is C_3, C_6, or a brush.*

5 The Characterization When $n = 3k + 2$

For this case $|A| = 0$, $|B| = |C| + 1$, and $|V - S| = |B| + m$. Since $n \geq 5$, we may assume $|D| = 0$ by Lemma 2. It follows as in the previous section that $m = 0$, $|V - S| = |B|$, $V - S = P_B$ and $V = C \cup B \cup P_B$. To deal with the fact that $|C| = |B| - 1$, we assume, without loss of generality, that $c_1 b_1$ and $c_1 b_2$ are edges, along with $c_i b_i$ for $i \geq 3$. Similar to the previous section, there are no edges from c_i to $B - \{b_1, b_2, b_i\}$ for any $i \geq 3$, there are no edges from v_i to $C \cup B - \{b_i\}$ for any i, and none of the vertices in B are adjacent to each other. Lemma 6 states that for each c_i, there must be at least one vertex, b_i which is adjacent to no vertex of $S - c_i$ so there are no edges from any b_i, $i \geq 3$ to c_1 and at most one of b_1 and b_2 can be adjacent to any c_j other than c_1. We assume, without loss of generality, that all such adjacencies are to b_1. Thus, in this case, the only edges in G that are not of the type c_ib_i or v_ib_i are those between vertices in C, between vertices in P_B, and from b_1 to $C - \{c_1\}$. Furthermore, b_i has degree two for $i \geq 2$.

The subgraph H induced by all vertices of the form c_i, b_i, and v_i for $i \geq 3$ satisfies the requirements of Corollary 5, so every component of H is C_6 or a brush. Suppose a component is a cycle, taken without loss of generality to be $(c_3, c_4, b_4, v_4, v_3, b_3, c_3)$. It must be joined to the subgraph J induced by c_1, b_1, b_2, v_1, and v_2. Corollary 4 assures there are no edges between either v_1 or v_2 and any v_j, $j \geq 3$. Furthermore, by Lemma 3, if $v_iv_j \in E$, $i, j \geq 3$, then c_i and c_j are not adjacent to either b_1 or c_1. Thus no component can be a cycle. It follows that any remaining edges of G involve only c_i's and b_1, except possibly for edge v_1v_2.

If edge v_1v_2 is present, $(v_1, b_1, c_1, b_2, v_2, v_1)$ forms a C_5. In this case, the C_5 must be the entire graph G, since a larger graph could be obtained only by joining the cycle to some c_j, $j \geq 3$, via an edge incident to c_1 or b_1. But then either $\downarrow (c_1, b_1, b_2 : v_1, v_2)$ or $\downarrow (c_1, b_1 : v_2)$. Thus, if $G \neq C_5$, $v_1v_2 \notin E$. This means all extremal graphs other than C_5 are constructed from the path $(v_1, b_1, c_1, b_2, v_2)$ by adding edges from b_1 and/or c_1 to an arbitrary number of vertices in the handles of an arbitrary number of brushes. This, along with a straightforward sufficiency check, is equivalent to the following characterization.

Theorem 8 *A connected graph G with $n = 3k+2$ vertices has $\gamma_t = \lfloor 2n/3 \rfloor$ if and only if G is C_5 or is obtained from a connected graph L by identifying an end vertex of a distinct P_3 with all but one vertex of L and identifying one vertex of a P_2 with the remaining vertex of L.*

6 The Characterization When $n = 3k + 1$

This section will show that each extremal graph when $n = 3k + 1$ has one of the forms shown in Figure 1. In this figure, a dotted edge indicates that that edge may or may not be present. If a form has two or more dotted edges, the text will clarify which ones must be in the graph under consideration. Any line between a vertex and a circled *br* indicates that the vertex may be adjacent to an arbitrary number of vertices in the handles of an arbitrary number of brushes. If the vertex is of type c_i, the brushes adjacent to it really form a single brush which includes the path (c_i, b_i, v_i). If two or more vertices have lines to the same circled *br*, it means that each of the vertices can be adjacent to an arbitrary number of vertices in the handles of an arbitrary number of brushes, including the same brushes as the other vertices and even the same vertices in the handles of those common brushes. In order to simplify the presentation, we have created classes in which there are a few overlaps. The characterization theorem to be proven is given next.

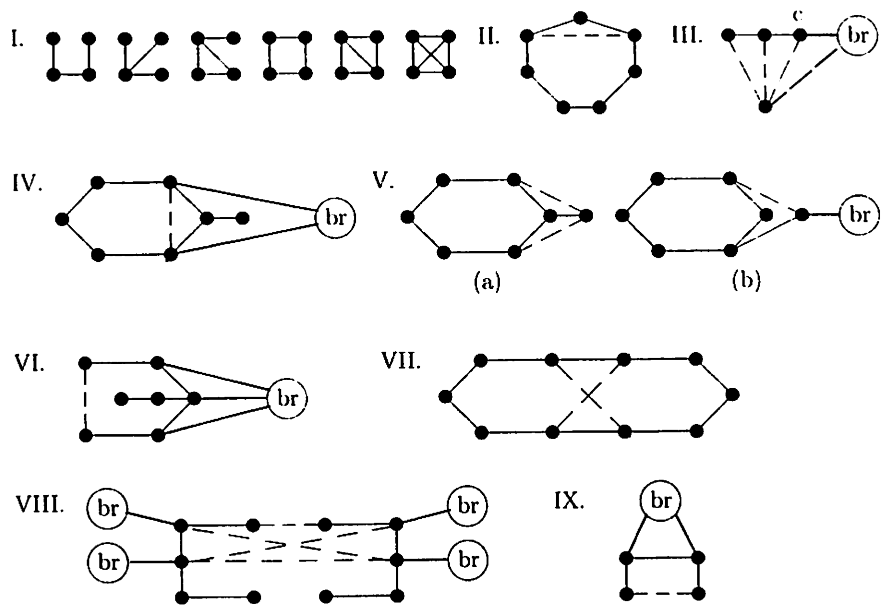

Figure 1.
The extremal graphs when $n = 3k + 1$,
with some dotted edges explained in the text

Theorem 9 *A connected graph G with $n = 3k+1$ vertices has $\gamma_t = \lfloor 2n/3 \rfloor$ if and only if G is one of the graphs depicted in Figure 1.*

A straightforward check shows that each of the graphs in Figure 1 is extremal. The six connected graphs shown as class I of the figure are the only extremal graphs on four vertices. All other extremal graphs will have at least seven vertices. To find them we consider the three subcases indicated in Section 3. Occasionally different subcases find the same graphs. We do not eliminate this duplication as it would obscure the fact that all subcases have been considered fully.

6.1 The Characterization When $|A| = 0$ and $|B| = |C|$

For this case we have $|S| = 2(|B| + m)$ and $|V - S| = |B| + m + 1$ so $V - S$ contains a private neighbor for each $b_i \in B$, a vertex adjacent to d_{i1} for each i in the range from 1 to m, and a single extra vertex z.

6.1.1 The General Structure

Consider the graph $G-z$ which has $3k$ vertices. Each component must contain at least three vertices since every vertex is in a not necessarily induced 3-path of the form (c_i, b_i, v_i) or (d_{i2}, d_{i1}, x_i). The choice of z indicates it is not the only private neighbor of any b_i. Hence, $2|B|$ vertices are needed to totally dominate the vertices in the (c_i, b_i, v_i) paths in $G-z$, and another $2m$ for the (x_i, d_{i1}, d_{i2}) paths. Thus, $\gamma_t(G-z) \geq 2(|B|+m) = \gamma_t(G)$. On the other hand, if $\gamma_t(G-z) > \gamma_t(G)$, z must be in every minimum total dominating set of G, which it is not. We conclude that $\gamma_t(G-z) = \gamma_t(G)$.

The next lemma shows that each component of $G-z$ is a cycle or a brush.

Lemma 10 *The components of $G-z$ are brushes, with the exception of at most one which is either a C_3 or a C_6.*

Proof: Suppose component i has $3k_i$ vertices for $1 \leq i \leq p$, $3k_i+1$ vertices for $p+1 \leq i \leq p+q$, and $3k_i+2$ vertices for $p+q+1 \leq i \leq p+q+r$. It follows that $\gamma_t(G-z) = \gamma_t(G) = 2k = 2\sum_{i=1}^{p+q+r} k_i + 2(q+2r)/3$ and, by considering the maximum possible total domination number for each of the components separately, $\gamma_t(G-z) \leq 2\sum_{i=1}^{p+q+r} k_i + r$. Thus we must have $r \geq 2(q+2r)/3$ which can be true only if $q = r = 0$, implying all components have a multiple of three vertices and have maximum possible total domination number. By Theorem 7, each component is C_3, C_6, or a brush.

Graph G is formed from the components by adding edges from the components to z. At most one of the components can be a cycle. If there are two cycles, z, a vertex adjacent to z on each of the cycles, and zero additional vertices for a C_3 and two for a C_6 permit a smaller total dominating set. □

Let us consider the possible edges from z to the components of $G-z$. If there is an edge between z and one of the end vertices of a P_3, we assume without loss of generality that the edge zc_i is present (where it is possible that zv_i also is an edge). On the other hand, if zv_i is an edge where v_i is a vertex of a nontrivial brush, c_i must be adjacent to another vertex in the handle of the brush. Combining these two facts, we see that, if z is adjacent to v_i, c_i must be adjacent either to z or to some c_j, $j \neq i$. If a component is a cycle, this observation leads to severe restrictions as to edges leading to z from brushes, as is shown in the following lemma.

Lemma 11 *If $G-z$ contains a component which is a cycle, then z is not adjacent to a b_i or a v_i in any brush.*

Proof: To see that zb_i cannot be an edge, note that the path (c_i, b_i, v_i) and the cycle would then be dominated by b_i, z, and one vertex of a C_3 or three of a C_6, resulting in a smaller total dominating set. On the other hand, if $zv_i \in E$, we have either c_ic_j or c_iz as an additional edge. In either case, the path and cycle are dominated by v_i, z, one vertex of a C_3 or three of a C_6, and c_j if c_ic_j is an edge, again causing a smaller total dominating set. □

Even if no component is a cycle, there still are additional restrictions on how z relates to the components.

Lemma 12 *Vertex z can be adjacent to at most one b_i and, if $(z, v_i, b_i, c_i, c_j, b_j, v_j, z)$ is not a cycle, at most one v_i.*

Proof: If zb_i and zb_j are edges, $\downarrow (c_i, c_j : z)$. Suppose zv_i is an edge. Recall that the corresponding c_i must have an adjacency to z or to a c_j. If $(z, v_i, b_i, c_i, c_j, b_j, v_j, z)$ is not a cycle, without loss of generality, either $c_jc_k \in E$ for $k \neq i, j$ or c_iz and c_jz are both edges. In either event, $\downarrow (b_i, b_j, c_j : z, v_j)$. □

6.1.2 The Graphs

We use the results from the previous subsection to generate the collection of graphs for this case. First, suppose $(z, v_i, b_i, c_i, c_j, b_j, v_j, z)$ forms a cycle. We show in this case that G must be one of the two graphs of II of Figure 1. It is easy to check that the cycle itself and the cycle with edge zb_i added are extremal. We cannot have an edge of the form zc_i since then $\downarrow (b_i, b_j : z)$. Recall v_iv_j is not an edge because the component containing v_i and v_j is a brush whose handle is composed of vertices of type c. Therefore, taking earlier restrictions into account, the only possible connections to other portions of the graph are between z, c_i, or c_j and a vertex $s \in S$. If $zs \in E$, $\downarrow (b_i, b_j : z)$ and, if $c_is \in E$ ($c_js \in E$ is similar), $\downarrow (b_i, b_j, c_j : z, v_j)$.

In all remaining cases, then, z is adjacent to at most one v_i and one b_j by Lemma 12. If $i = j$ and z is adjacent to both v_i and b_i, we have the structure of Figure 2 where c_i is adjacent either to z or some c_k. Here z is not adjacent to any other c_j, for in such a situation $\downarrow (b_i, c_i : z)$. Thus there is only one component of $G - z$ and all graphs of this form are constructed from a single brush with the edges zv_i and zb_i incident to one of the P_3's of the brush. The edge zc_i may or may not be present. These are precisely the graphs III of Figure 1 where the leftmost two dotted edges are present and the dotted line representing possible edges to brushes is not present. The remaining dotted edge may or may not be present. There is at least one brush since the graph has at least seven vertices.

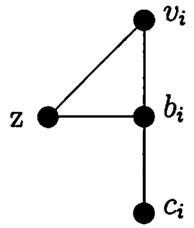

Figure 2. Basic structure leading to the graphs III of Figure 1

If at most one of zv_i or zb_i is an edge and there are no edges from z to v_j or b_j, $j \neq i$, then the graphs formed by connecting c_i and/or z to arbitrarily many brushes are all extremal. The edge zc_i may or may not be present. These again are the graphs III of Figure 1 where at least one of the leftmost dotted edges is missing.

Now suppose $i \neq j$ and zv_i, $zb_j \in E$. If c_iz or c_ic_k is an edge with $k \neq j$, then $\downarrow (b_i, c_i, c_j : z, v_i)$. Since c_i must be adjacent to either z or some c_k, the only remaining possibility is that c_ic_j is an edge and c_i must have degree two in G. Thus any extremal graphs to be found under this situation must contain the structure shown in Figure 3 and be formed by joining c_j and/or z to brushes. The edge zc_j may or may not be present. These are the graphs IV of Figure 1.

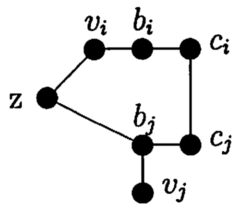

Figure 3. Basic structure leading to the graphs IV of Figure 1

In the only remaining case, z is not adjacent to either a v_i or a b_j. By Lemma 11 this is the only case for which a cycle can be joined to z. If z is not connected to a cycle, we have the graphs III of Figure 1 with both of the leftmost edges missing. If z is connected to a C_3, we again have the graphs III but with the vertex labeled c relabeled as z and the dotted edge to the brush missing. Notice that z can be adjacent to at most two vertices of the C_3. The remaining situations are graphs V of Figure 1 in which z is adjacent to a C_6. If G is the graph induced by z and the vertices of the C_6, it is easy to see that G must be one of the graphs of V(a). If G has more than seven vertices, the C_6 can be joined to z by at most two edges, and then only if the two vertices of the cycle which are involved are distance two apart, which produces the graphs of V(b).

6.2 The Characterization When $|A| = 0$ and $|B| = |C| + 2$

For this case $|S| = 2(|B| - 1 + m)$ and $|V - S| = |B| + m$. By Lemma 2 we may assume $m = 0$. Since $|B| = |C| + 2$, one of the structures depicted in Figure 4 must be present in any extremal graph. Furthermore, $c_i b_i$ is an edge for $i \geq 4$ when structure (a) appears and for $i \geq 5$ when structure (b) does, and each such b_i is adjacent to no other c_j by Lemma 6.

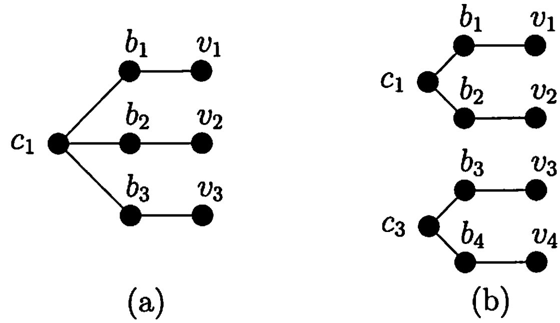

Figure 4. Basic structures for the graphs of Section 6.2

Corollary 4 shows there is no edge $v_i v_j$ when $i \leq 3$ and $j \geq 4$ if structure (a) is used and when $i \leq 4$ and $j \geq 5$ if structure (b) is used. Thus the structures of Figure 4 cannot be joined to the rest of the graph by edges involving v_1, v_2, v_3, or v_4. Lemma 6 indicates, without loss of generality, that the only b_i's from the structure (a) which can be adjacent to other c_j's are b_1 and b_2. It also shows that only one of b_1 and b_2 and one of b_3 and b_4 can be so joined. However, it is convenient not to pin down which of these can have the adjacencies because it depends on how the two parts of structure (b) are joined to each other.

Let us first concentrate on structure (a). If there are at least two edges between v_1, v_2, and v_3, say v_1v_2 and v_2v_3, then $\downarrow (b_1, b_3 : v_2)$. If $v_1v_3, b_2c_j \in E$ where $j \geq 4$, then $\downarrow (c_1, b_1, b_3 : v_1, v_3)$. From this it can be concluded, since we are assuming that only b_1 and b_2 can have edges to c_j's other than c_1, that, if there is any edge between v_1, v_2, and v_3, it can always be taken to be v_1v_2. The graphs permitted by these restrictions are obtained from structure (a) by connecting any of c_1, b_1, and b_2 to brushes. The edge v_1v_2 may or may not be present. These are the graphs represented by VI in Figure 1.

All remaining extremal graphs must contain structure (b). First consider the way edges can exist among the four v vertices of the structure. If $v_1v_2 \in E$, a C_5 is formed. This cannot be the entire graph since $n = 3k+1$, so it must be joined to the rest of the graph either by an edge between at least one of b_1, b_2, and c_1 and some vertex $s \in S$ or by edges between v_1 or v_2

and v_3 or v_4. If $c_1 s \in E$, $\downarrow (c_1, b_1, b_2 : v_1, v_2)$; if $b_1 s \in E$, $\downarrow (b_1, c_1 : v_2)$; and if $b_2 s \in E$, $\downarrow (b_2, c_1 : v_1)$. Finally if, for example, $v_1 v_3 \in E$, $\downarrow (b_2, b_3 : v_1)$. We conclude that $v_1 v_2, v_3 v_4 \notin E$. We now consider all possible connections between the pair v_1 and v_2 and the pair v_3 and v_4.

Suppose a C_{10} is formed, for example when $v_1 v_3$ and $v_2 v_4$ are edges. Possible graphs obtained this way are illustrated by the graphs VII of Figure 1. We will show these are the only possibilites. Observe first there can be no additional internal edges. If there were one, it would have to be equivalent either to $c_1 b_3$, or to $c_1 c_3$. In the former case, $\downarrow (c_3, b_1, b_2, b_4 : v_2, v_3, v_4)$. In the latter, if either dotted edge is present, say $v_1 v_4$, along with $c_1 b_3$, $\downarrow (b_1, b_2, b_3, b_4 : v_1, v_2, v_4)$ and if neither dotted edge exists, then c_1 relabeled as v_1 and c_3 relabeled v_4 results in one of the graphs of VII. It also is not possible to join the cycle to vertices outside it, for then there would have to be an edge between a vertex x of the cycle and a vertex $s \in S$ external to the cycle. But then s dominates x and the other nine vertices of the cycle are dominated by only five vertices of the cycle, thereby reducing the size of S by one, a contradiction.

Any remaining graphs have at most two edges joining v_1 and v_2 to v_3 and v_4 and, without loss of generality, we may assume any such edges are incident to v_1.

When there are two joining edges, the structure must be equivalent to that of Figure 5. By relabeling b_1 as z, v_3 as a b and b_3 as a c, we have a situation considered in Section 6.1 which led to the graphs V(b) of Figure 1.

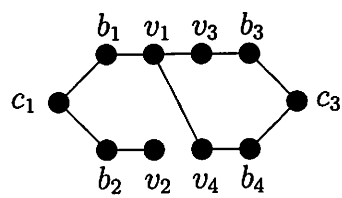

Figure 5. Basic structure for graphs in class V(b) of Figure 1

The last cases involve either the single edge $v_1 v_3$ or no edges, as illustrated in Figure 6. When $v_1 v_3$ is present, edges $c_1 c_3$, $c_1 b_3$, and $c_3 b_1$ are possible. However $c_1 b_4$ (and $c_3 b_2$ by similarity) is not possible since then $\downarrow (b_1, c_3 : v_3)$. There also can be no edge from b_2 (or b_4) to a vertex $s \in S$ external to the structure for then $\downarrow (b_1, b_3, c_1 : v_1, v_3)$. A similar argument can be given when there are no edges between the v vertices of structure (b) in Figure 4. Again we cannot have both of the edges $c_1 b_3$ and $c_1 b_4$, for then $S - \{c_3\}$ is a smaller total dominating set. Similarly both of the edges $c_3 b_1$ and $c_3 b_2$ cannot be present. Therefore all possible graphs are obtained from the structures of Figure 6 by joining b_1, b_3, c_1, and c_3 to brushes, with edges c_1c_3, c_1b_3, and c_3b_1 allowed. These are the graphs VIII of Figure 1 where at least one of the dotted edges must be present.

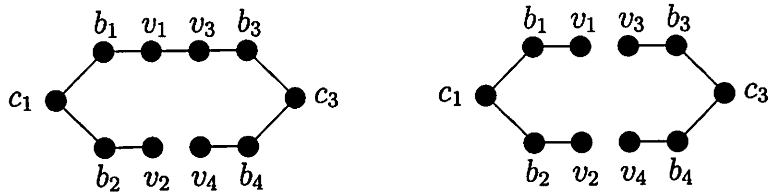

Figure 6.
Basic structures leading to the graphs in class VIII of Figure 1

6.3 The Characterization When $|A| = 2$

Here $|B| = |C|$, $|S| = 2|B| + 2 + 2m$, and $|V - S| = |B| + m + 2$ and all graphs of concern here contain the path (w_1, a_1, a_2, w_2). We may assume that th degree of a_1 is at least three. Suppose it is two. Then we may relabel a_1 as a b and one of w_1 and a_2 as the corresponding c and the other as the corresponding v, depending on the structure of the rest of the graph. Then we have the requirements leading to the situation in Section 6.1 with w_2 corresponding to z. Similarly, the degree of a_2 is at least three. These restrictions and the following observation show the number of cases that need to be considered is severely limited.

Observation 13 *The edges w_1v_i and a_2c_j (w_2v_i and a_1c_j) cannot both occur if $i \neq j$.*

Proof: If w_1v_i and a_2c_j are edges, $\downarrow (a_1, c_i : v_i)$. □

It follows that the only possible additional edges involving w_1 and w_2 are w_1w_2, and w_1v_i if a_2c_i also is an edge (w_2v_i if a_1c_i also is an edge).

If neither w_1v_i nor w_2v_i is an edge, all graphs are obtained from the 4-path by connecting a_1 and/or a_2 to brushes, where edge w_1w_2 may or may not be present. This leads to the graphs IX of Figure 1.

The next situation is when we have the structure of Figure 7. The edge w_1w_2 may be present or absent. By Observation 13, nothing else can be adjacent to either a_1 or w_2, and only one of w_1 and a_2 can have additional adjacencies. Thus the only possible graphs are those which are obtained from the structure of Figure 7 by joining w_1 to brushes, creating some of the graphs V(b) of Figure 1, or by joining a_2 to brushes, creating some of the graphs IV of that figure.

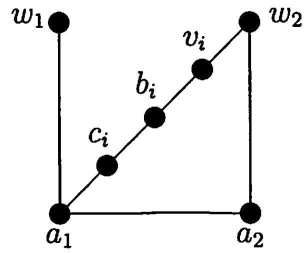

Figure 7.
Basic structure leading to graphs in classes IV and V(b) of Figure 1

The only other possibility is depicted in Figure 8. Observation 13 indicates that nothing can be added to this graph, so it must be all of G and is one of the graphs VII of Figure 1.

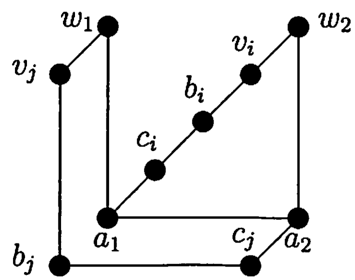

Figure 8. A graph in class VII of Figure 1

6.4 Summary

The results of the previous three subsections complete the proof of Theorem 9.

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