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Domination and Power Domination in Certain Families of Nanostars Dendrimers

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ABSTRACT Dendrimers are hyper-branched macromolecules having various applications in diverse fields like supra-molecular chemistry, drug delivery and nanotechnology etc. The certain graph invariants such as dominating number and power dominating number can be used to characterize large number of physical properties like physio-chemical properties, thermodynamic properties, chemical and biological activities, etc. A subset of a simple undirected graph is called dominating set if every vertex of the given graph is either in that set or is adjacent to some vertex in that set. The minimum number of elements in that kind of set is called domination number. A subset of the vertex set of a graph G is said to be power dominating set (PDS) of G, if every vertex and every edge in G is observed by P. The minimum cardinality of P of a graph G is called power domination number. In this paper, the domination number and power domination number of some nanostars dendrimers have been determined.

INDEX TERMS Domination number, power domination number, dendrimers.

I. INTRODUCTION

A dendrimer is a molecule that is manufactured artificially and it has well defined chemical structure. The structure of dendrimers are composed by three major architectural components: one component is core which is the basic component in construction of dendrimer, then branches which added in each step recursively to create a tree like structure and finally, the end groups. The nanostar dendrimer behaves as macroparticles which appear to be photon funnels and is like artificial antennas.

Let G be simple and undirected graph with vertex set V and edge set E. A dominating set is a subset of the vertex set of G such that every vertex in $V(G) - D$ is adjacent to at least one member of D. The smallest number of elements in D is called the dominating number of G and is denoted by $\gamma = \gamma(G)$.

The dominating number is an extensively studied graph invariants in graph theory. The domination number are obtained for grids [7], for regular graphs [6], for cartesian product of directed cycles, the cartesian products of two directed paths, the cartesian product of the cycle of length n [9], [11], [19].

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For any vertex v of G, the open neighbor hood is the set of all elements which are connected to v. The closed neighborhood of v is the union of set of all elements connected to v and the element v. Mathematically, we define: $N(v) = \{u \in V(G) : vu \in E(G)\}$ and $N[v] = \{v\} \cup N(v)$ respectively. For a set $P \subseteq V$, let $N(P) = \cup_{V \in P} N(V) - P$ is the open neighborhood and $N[P] = N(P) \cup P$ be the close neighborhoods of P.

A subset P of the vertex set is said to be a power dominating set (abbreviated as PDS) if every vertex and every edge in G is observed by P. The set observed by P is denoted by $M(P)$. A PDS of G with the minimum cardinality is called power domination number and is denoted by $\gamma_P(G)$. It is obvious to note that every dominating set is a PDS. The PDS is constructed as follows:

(1) First write those vertices into $M(P)$ which are in closed neighborhood of P.

(2) Add all vertices w in $M(P)$ which are adjacent to v which is already in $M(P)$ such that all the other vertices which are adjacent to v are already in $M(P)$. When there is no such vertex w exists, then the set mentioned by P is constructed.

The Phase Measurement Unit (PMU) is used to measure the voltage of node and current phase of the edges connected to the node in electric power network. These problems are

solved by installing the minimum number of *PMUs* such that the whole system is monitored.

In the study of mathematical chemistry, a molecular graph or chemical graph is a representation of the structural formula of a chemical compound in terms of graph theory. A chemical graph is a labeled graph whose vertices correspond to the atoms of the compound and edges correspond to chemical bonds. Many chemical structures such as Sierpinski networks [13], silicate networks [10] were modeled as graphs and studied. Upper bounds on the power domination are given for different graphs in [2], [4], [20] and the power domination number of various graphs are studied in [2], [3], [5], [8], [16].

In this article, we study the domination and power domination for complex chemical networks like some infinite families of Nanostar Dendrimers. We derive the exact values of domination and power domination for these classes of complex chemical networks.

II. PRELIMINARY RESULT

A well known power domination subgraph relation is introduced by Sudeep Stephen in [15], which is stated as

Theorem 2.1 (Power Domination-Subgraph Relation): Let $K_1, \ldots, K_r$ are subgraphs of G such that $K_i \cap K_j = \phi$ and fulfill the two conditions stated below:

1. $V(K_i) = V_1(K_i) \cup V_2(K_I)$ where $V_1(K_i) = \{x \in V(K_i) | x \sim y for some\ y \in V(G) - V(K_i)\}$ and $V_2(K_i) = \{x \in V(K_i) | x \nsim y for all\ y \in V(G) - V(K_i)\}$.
2. $V_2(K_i) \neq \phi$ and for each $x \in V_1(K_i)$, there are at least two vertices in $V_2(K_i)$ which are connected to x.

If $V_1(K_i)$ is observed and if l_i are minimum number of vertices which are required to observe vertex set of each K_i, then $\gamma(G) \geq \Sigma_{i=1}^{k} l_i$.

III. THE GRAPH OF FIRST KIND OF DENDRIMER $D_1[n]$

We denote in this section the molecular graph $D_1[n]$ defined in [3] by $G(n)$, where n denotes the step of growth. Suppose $G(0)$ and H are the graphs obtained by the vertex gluing of a hexagon C_6 with K_2 and P_4, respectively. The graph $G(0)$ is called the core of the graph $G(n)$ and H is the graph of added branch. The structure of graph $G(n) = D_1[n]$ is constructed by adding 2^k, $1 \leq k \leq n$ copies of added branch H at each step. Figure 1 depicts the graph of $G(2)$ with two growth stages. Moreover, it can be observe that, $V(G(n)) = 2^{n+4} - 9$ and $E(G(n)) = 18 \times 2^n - 11$.

Definition 3.1: The number of non-hexagon edges incident at its vertices is the degree of a hexagon.

Theorem 3.1: If G be the graph of first kind of dendrimer $D_1[n]$. Then $\gamma(G) = 5.2^n - 3$, for $n \geq 1$.

Proof: Let H_i and K_j be the graphs obtained by joining the vertices of G which are adjacent to the hexagons of degree 3 and degree 1 respectively. By the construction of graph G, the subgraphs H_i and K_j are pairwise disjoint. Since we have $2^n - 1$ copies of H_i and 2^n copies of K_j. Therefore, there must exist at least one vertex from each copy of the graph H_i and K_j which belong to the dominating set. Thus $\gamma(G) \geq \Sigma_{i=1}^{2^n-1}\gamma(H_i) + \Sigma_{j=1}^{2^n}\gamma(K_j) = 5.2^n - 3$.

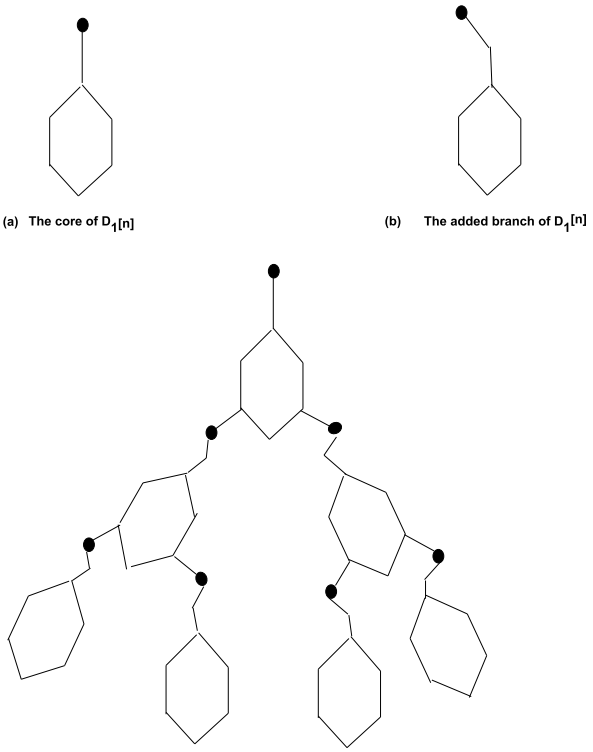

FIGURE 1. The structure of the graph of $D_1[n]$.

Since, the graph G has 2^n hexagons of degree one. Let $y_1, y_2, \ldots, y_{2^n}$ be the end vertices of each hexagon. Define the dominating set as follows:

$D = \{x \epsilon\ G : deg(x) = 3\} \cup \{y_i : 1 \leq i \leq 2^n\}$. Thus $|D| = 2^n + 4.2^n - 3 = 5.2^n - 3$. This implies that $\gamma(G) \leq 5.2^n - 3$.

Theorem 3.2: If G be the graph of first kind of dendrimer $D_1[n]$. Then $\gamma_P(G) = 2^{n+1} - 1$, for $n \geq 1$.

Proof: Let us denote the hexagons in the graph $D_1[n]$ by H_i. From the construction of the graph, $D_1[n]$ has $2^{n+1} - 1$ hexagons. Let $X = \{H_i : H_i\ is\ Hexagon\ in\ D_1[n]\}$. Then $|X| = 2^{n+1} - 1$. Since each hexagon H_i is observed by a single vertex. Therefore, by Theorem [15], $l_i = 1$, we have $\gamma_p(G) \geq 2^{n+1} - 1$.

On the other hand, every vertex of degree 3 in each of the hexagon observe all other vertices in that hexagon. Let Y be a set which contains at least one vertex of degree 3 in each of the hexagon. Then $\gamma(G)_p \leq 2^{n+1} - 1$.

IV. THE GRAPH OF THIRD KIND OF DENDRIMER $D_3[n]$

In this section, the domination number and power domination number of the graph of third kind of dendrimer $D_3[n]$ defined in [3] is discussed. In this type of dendrimers, the core consists of three hexagons. The graph $G(n) = D_3[n]$ is constructed by adding 3.2^k $(1 \leq k \leq n)$ copies of the graph of added branch H at each step. The structure of this type of dendrimers with two growth stages, $D_3[2]$ is shown in Figure 2. From the construction of graph, we have $|V(D_3[n])| = 42.2^n - 20$ and $|E(D_3[n])| = 48 \times 2^n - 24$.

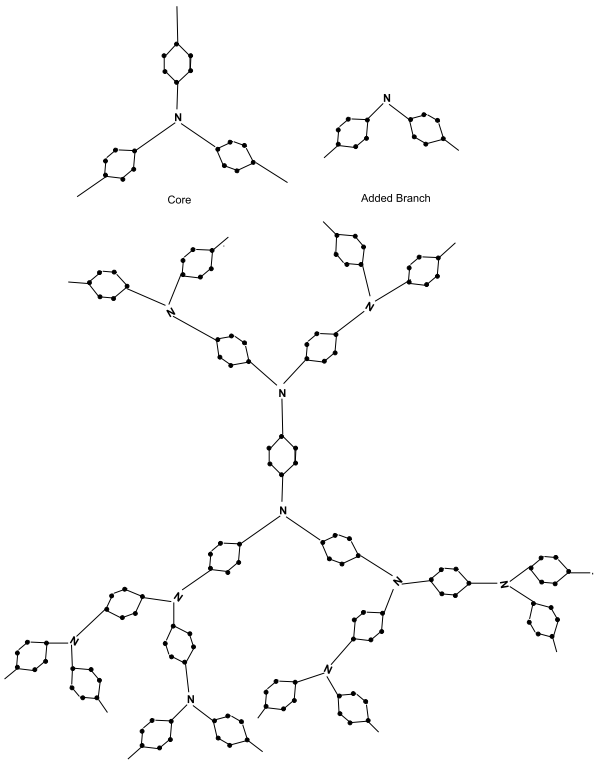

FIGURE 2. The structure of the graph $D_3[2]$.

Theorem 4.1: If G be the graph of $D_3[n]$. Then $\gamma(G) = 6(2^{n+1} - 1)$, for $n \geq 0$.

Proof: Let us denote the hexagons in the graph $D_3[n]$ by H_i. From the construction of the graph, $D_3[n]$ has $3(2^{n+1} - 1)$ hexagons. Let $X = \{H_i : H_i \text{ is Hexagon in } D_3[n]\}$. Then $|X| = 3(2^{n+1} - 1)$. Therefore, there must exist at least two vertices from each copy of the graph H_i which belong to the dominating set. It yields that $\gamma(G) \geq \Sigma_{i=1}^{3(2^{n+1}-1)}\gamma(H_i) = 6(2^{n+1} - 1)$.

Since the graph G has $3(2^{n+1} - 1)$ hexagons of degree two. Define the dominating set as follows $D = \{x\epsilon\ G : deg(x) = 3\}$. Now $|D| = 2(3(2^{n+1} - 1)) = 6(2^{n+1} - 1)$. This implies that $\gamma(G) \leq 6(2^{n+1} - 1)$.

Theorem 4.2: If G be the graph of third kind of dendrimer $D_3[n]$. Then $\gamma_P(G) = 3.2^{n+1} - 3$ for $n \geq 0$.

Proof: Let us denote the hexagons in the graph $D_3[n]$ by H_i. From the construction of the graph, $D_3[n]$ has $3(2^{n+1} - 1)$ hexagons. In this graph degree of each hexagon is 2. Let $X = \{H_i : H_i \text{ is Hexagon in } D_3[n]\}$. Since each hexagon H_i is observed by a single vertex. Therefore, by Theorem 2.1, $l_i = 1$, therefore $\gamma_p(G) \geq 3.2^{n+1} - 3$.

Now to prove the upper bound, we construct a power dominating set of cardinality $3.2^{n+1} - 3$. Every vertex of degree 3 in each hexagon observe all other vertices in that hexagon. Let Y be a set which contain at least one vertex of degree 3 in each of the hexagon. Then $\gamma_p(G) \geq 3.2^{n+1} - 3$.

V. THE GRAPH OF NANOSTAR DENDRIMERS

The molecular graph of a nanostar dendrimer $NS[n]$ is defined in [1] with exactly n generations. Consider the core of $NS[n]$ and the graph with one generation $NS[1]$ are depicted in Figure 3. The graph $NS[n]$ is constructed by adding 3.2^k $(1 \leq k \leq n)$ copies of the graph of added branch H at each step. Obviously, $|V(NS[n])| = 12(3.2^n - 1)$ and $|EV(NS[n])| = 42.2^n - 15$. The domination number and power domination of nanostar dendrimer are discussed in this section.

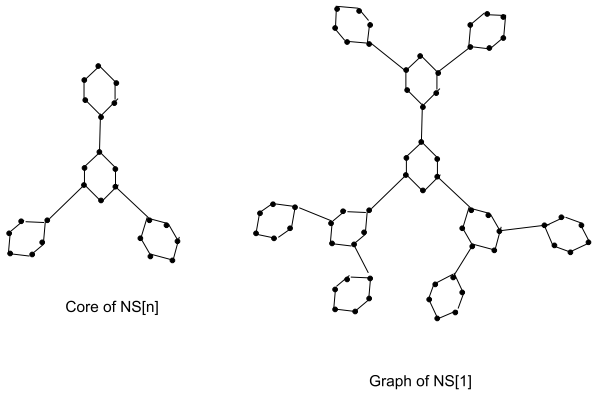

FIGURE 3. The graph $NS[1]$ with one generation.

Lemma 5.1: If G be the graph of nanostar dendrimer $NS[n]$. Then $\gamma(G) \geq 2(6.2^n - 2)$, for $n \geq 0$.

Proof: Let D be a dominating set for the graph G. Since G has $6.2^n - 2$ hexagons, therefore it is enough to show that the dominating set$D$ contain at least two vertices from each hexagon. Let H be an arbitrary hexagon in G with vertex set $V(H) = \{l_1, l_2, l_3, p_1, p_2, p_3\}$, where $deg(l_i) = 3$. It is important that the vertices l_1, l_2, l_3 connect the graph H to the remaining graph. Now we have two cases.

Case 1: $N(D) \cap V(H) = \emptyset$

Since any vertex in H can dominate at most three vertices of H. Therefore D contain at least two vertices of the graph H.

Case 2: $N(D) \cap V(H) \neq \emptyset$

In this case l_1, l_2, l_3 can only belong to $N(D)$. To dominate the vertices p_1, p_2 *and* p_3, at least one vertex from the set of vertices $\{p_1, l_1, p_2\}$ and $\{l_2, p_3, l_3\}$ must belong to D. Therefore $\gamma(G) \geq 2(6.2^n - 2)$.

Lemma 5.2: If G be the graph of nanostar dendrimer $NS[n]$. Then $\gamma(G) \leq 2(6.2^n - 1)$, for $n \geq 0$.

Proof: Let H be the graph of the added branch. Let D be the dominating set consisting of the vertex (*say* x) which has degree 3 in H and the vertex which is at distance 3 from x. $D = \{x\epsilon\ H : deg_H(x) = 3\} \cup \{y\epsilon\ H : d(x, y) = 3\}$. Since there are $(6.2^n - 2)$ are edge disjoint copies of H, therefore $\gamma(G) \leq 2(6.2^n - 2)$.

From Lemma 5.1 and Lemma 5.2, we can state the following main theorem.

Theorem 5.3: For $n \geq 0$, $\gamma(G) = 2(6.2^n - 1)$.

Theorem 5.4: If G is the graph of Nanostar dendrimer $NS[n]$. Then $\gamma_P(NS[n]) = 2(3.2^n - 1)$, for $n \geq 0$.

Proof: The molecular graph of nanostar dendrimer has hexagons of degree 3 and 1. The hexagons of degree 1 lie only in n^{th} generation. Let X be the collection of all hexagons of degree 3 and 1. Thus $|X| = 2(3.2^n - 1)$. Since each hexagon H_i is observed by a single vertex, Therefore, Theorem 2.1, $l_i = 1$. Hence, $\gamma_P(G) \geq 2(3.2^n - 1)$. To prove $\gamma_P(G) \leq 2(3.2^n - 1)$, we construct a power dominating set of cardinality $2(3.2^n - 1)$. Let Y be the set constructed by taking one vertex from each hexagon H_i. i.e $Y = \{x_i \in V(H_i) : i = 1, 2, 3, \ldots, 2(3.2^n - 1)\}$. It is easy see that set Y observed thee all vertices of $NS[n]$.

VI. THE GRAPH OF TREE DENDRIMER

Consider the graph of tree dendrimer $T_{l,p}$ known as regular dendrimer defined in [18]. Let v_0 be the center of the graph of $T_{l,p}$. The degree of every non-pendant vertex is p and the distance between every pendant vertex and the central vertex v_0 is l. $T_{2,3}$ and $T_{3,4}$ are shown in following figure.

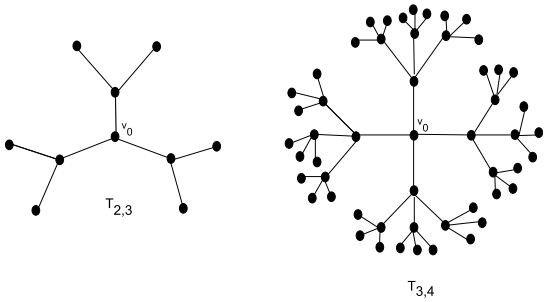

FIGURE 4. The graph of tree dendrimer $T_{2,3}$ and $T_{3,4}$.

Theorem 6.1: For $l, p \geq 2$,

$$\gamma(T_{l,p}) = \begin{cases} 1 + \dfrac{p(p-1)[(p-1)^l - 1]}{(p-1)^3 - 1}, & \text{if } l \equiv 0(mod3) \\ 1 + \dfrac{p(p-1)^2[(p-1)^{l-1} - 1]}{(p-1)^3 - 1}, & \text{if } l \equiv 1(mod3) \\ p\dfrac{(p-1)^{l+1} - 1}{(p-1)^3 - 1}, & \text{if } l \equiv 2(mod3) \end{cases}$$

Proof: Let D be a dominating set and $f(s)$ be the number of vertices of the graph $T_{s,p}$ in D. It is worthy to see that the graph of $T_{s,p}$ can be obtained from the graph of $T_{s-1,p}$ by adding $p(p-1)^{l-2}$ $(2 \leq s \leq l)$ copies of the added branch H. Since the graph H is isomorphic to $K_{1,s-1}$. Therefore to dominate the pendant vertices there must exist at least one vertex in D from each copy of the graph H. Also no vertex in the graph $T_{s-3,p}$ can dominate any vertex of the graph $T_{s,p}$. Now we have the following three cases.

Case 1: If $p \equiv 0(mod3)$.

This case implies that $f(s) \geq f(s-3) + p(p-1)^{3s-2}$. By backward substitution

$$f(T_{s,p}) \geq f(T_{3,p}) + p[(p-1)^4 + (p-1)^7 + \ldots + (p-1)^{l-2}]$$

Since $f(T_{3,p}) \geq 1 + p(p-1)$, so

$$f(T_{s,p}) \geq 1 + p[(p-1)^1 + (p-1)^4 + (p-1)^7 + \ldots + (p-1)^{l-2}],$$

from above it is concluded that

$$f(T_{l,p}) \geq 1 + \frac{p(p-1)[(p-1)^k - 1]}{(p-1)^3 - 1}.$$

Case 2: If $p \equiv 1(mod3)$.

This case implies that $f(s) \geq f(s-3) + p(p-1)^{3s-1}$. By backward substitution

$$f(T_{s,p}) \geq f(T_{4,p}) + p[(p-1)^5 + \cdots + (p-1)^{l-2}]$$

Since $f(T_{4,p}) \geq 1 + p(p-1)^2$, so

$$f(T_{s,p}) \geq 1 + p[(p-1)^2 + (p-1)^5 + \ldots + (p-1)^{l-2}],$$

this conclude that

$$f(T_{l,p}) \geq 1 + \frac{p(p-1)^2[(p-1)^{l-1} - 1]}{(p-1)^3 - 1}.$$

Case 3: If $p \equiv 2(mod3)$.

This case implies that $f(s) \geq f(s-3) + p(p-1)^{3s-3}$. By backward substitution

$$f(T_{s,p}) \geq f(T_{2,p}) + p[(p-1)^3 + (p-1)^6 + \ldots + (p-1)^{l-2}]$$

Since $f(T_{2,p}) \geq p$, so

$$f(T_{s,p}) \geq p + p[(p-1)^3 + (p-1)^6 + \ldots + (p-1)^{l-2}],$$

this conclude that

$$f(T_{l,p}) \geq p\frac{(p-1)^{l+1} - 1}{(p-1)^3 - 1}.$$

To prove the upper bounds in above three cases, we proceed as follows:

Case 1: If $p \equiv 0(mod3)$

Consider the set $D_1 = \{x \in G \mid d(x, v_0) = 3l - 1, \forall\ 1 \leq l \leq \frac{l}{3}\} \cup \{v_0\}$.

Since the graph $T_{l,p}$ has l-stages. If $p \equiv 0(mod3)$, then in each stage there are $p(p-1)^{3s-2}$ vertices which are at distance $3s-1$ from v_0. Therefore $|D_1| = 1 + \frac{p(p-1)[(p-1)^l - 1]}{(p-1)^3 - 1}$

Case 2: if $p \equiv 1(mod3)$

Consider the set $D_2 = \{x \in G | d(x, v_0) = 3l, \forall\ 1 \leq l \leq \frac{l-1}{3}\} \cup \{v_0\}$.

In this case there are $p(p-1)^{3s-1}$ vertices which are at distance $3s$ from v_0. Therefore $|D_2| = 1 + \frac{p(p-1)^2[(p-1)^{l-1} - 1]}{(p-1)^3 - 1}$.

Case 3: If $p \equiv 2(mod3)$

Consider the set $D_3 = \{x \in G | d(x, v_0) = 3l - 2, \forall\ 1 \leq l \leq \frac{l+1}{3}\}$

Since there are $p(p-1)^{3s-3}$ vertices which are at distance $3s-2$ from v_0 in each stage. Therefore $|D_3| = p\frac{(p-1)^{l+1} - 1}{(p-1)^3 - 1}$.

All above cases implies that all the vertices of the graph $T_{l,p}$ are dominated. Hence

$$\gamma(T_{l,p}) = \begin{cases} 1 + \dfrac{p(p-1)[(p-1)^l - 1]}{(p-1)^3 - 1}, & \text{if } p \equiv 0(mod\ 3) \\ 1 + \dfrac{p(p-1)^2[(p-1)^{l-1} - 1]}{(p-1)^3 - 1}, & \text{if } p \equiv 1(mod\ 3) \\ p\dfrac{(p-1)^{l+1} - 1}{(p-1)^3 - 1}, & \text{if } p \equiv 2(mod\ 3) \end{cases}$$

Theorem 6.2: $\gamma_P(T_{l,p}) = p(p-1)^{l-2}$, for $l \geq 2$ and $p \geq 2$.

Proof: Let us denote all the star graphs in $T_{l,p}$ by H_i which are isomorphic to $K_{1,\,s-1}$. These star graphs are at distance l from the central vertex v_0. The degree of the central vertex in H_i is p. Let $X = \{H_i : H_i \text{ is isomorphic to } K_{1,\,s-1} \text{ in } T_{l,p}\}$, where $|X| = p(p-1)^{l-2}$. Since each H_i is observed by a single vertex, therefore $s_i = 1$. By theorem, we have $\gamma_P(T_{l,p}) \geq p(p-1)^{l-2}$. Now to prove upper bound, we exhibit a power dominating set of cardinality $p(p-1)^{l-2}$. Let Y be a set which contain at least one vertex of degree $p-1$ in each of H_i. Then $\gamma_P(T_{l,p}) \leq p(p-1)^{l-2}$. It is easy to see that set Y observed all the vertices of $T_{l,p}$.

VII. CONCLUSION

Domination and power domination problem is graph theory is widely studied problem. It has many applications in different areas. In this work, domination and power domination number problem for some infinite classes of Nanostar Dendrimers are explored and exact values of these parameters have been computed. We believe that these results will be helpful for people working in that filed to understand and predict the physio-chemical properties for these chemical structures.

In future, we are interested to identify more such chemical structures and compute their domination and power domination number and other graph parameters to explore more physical chemical properties.

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