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On The Second Domination Hyper Polynomial of Graphs

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Abstract

Graph polynomials are powerful and well-developed tools to express graph parameters. A chemical graph can be recognized by a numerical number (topological index), algebraic polynomial, or any matrix. These numbers and polynomials help to predict many physicochemical properties of underline chemical compounds. In this paper, we define a new version of domination polynomials known as the second domination hyper polynomial. Also, we will study and calculate this new polynomial for some graph families. Also, we calculate the second domination hyper polynomials with its plotting for Hexane isomers.

Keywords: Second domination hyper index; Domination degree; Minimal domination set; Second domination hyper polynomial.
2020 Mathematics Subject Classification: 05C69, 05C10.

1. Introduction

Chemical Numerous graph polynomials are available in the recent literature and several among them are applicable in mathematical chemistry. Graph polynomials are powerful and well-developed tools to express graph parameters. In this paper, we assume that Φ is a connected graph without loops. With the vertex set $V(\Phi)$ and edge set $E(\Phi)$. There are two classified topological indices generally into two kinds: degree-based indices, and distance-based indices. In this paper, we assume that Φ is a connected graph without loops. With the vertex set $V(\Phi)$ and edge set $E(\Phi)$. The degree $d(v)$ of a vertex v in graph Φ is defined as the number of first neighbors of vertex v in Φ. The concept of degree in graph theory is closely related to the concept of valence in chemistry. The complement of a graph Φ, represented through $\overline{\Phi}$, is a simple graph on the similar set of vertices $V(\Phi)$ where two vertices u and v are joined by an edge uv, if and only if they are not adjacent in Φ. The second hyper domination index defined as follows:

$$DHZ_2(\Phi) = \sum_{fg \in E(\Phi)} (d_{df} d_{dg})^2.$$

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We can list some major of topological indices such as degree-based-topological indices and distance based-topological indices see [11–13]. For more discussion, see [1,3,10,29,35–37]. A graph Φ is called connected if there is a path between any two vertices of Φ. Otherwise, Φ is called disconnected. A set $S \subseteq V(\Phi)$ is called a dominating set of Φ, if for any vertex $f \in V(\Phi) - S$ there exists a vertex $g \in S$ such that f and g are adjacent. A dominating set $S = \{f_1, f_2, ..., f_r\}$ is minimal domination set if $S - f_i$ is not a dominating set. In [34], the authors used the notation $\Upsilon_m(\Phi)$ to denote the number of minimal domination sets. In [14,34] (2021) Hanan Ahmed et al, have defined a new polynomials based on minimal dominating sets called domination Zagreb polynomials and they are defined as follows:

$$DM_1(\Phi,x) = \sum_{f\in V(\Phi)} x^{d_{df}^2}, \qquad DM_2(\Phi,x) = \sum_{fg\in E(\Phi)} x^{d_{df}d_{dg}}$$
$$DM_1^*(\Phi,x) = \sum_{fg\in E(\Phi)} x^{[d_{df}+d_{dg}]}, \qquad DF(\Phi,x) = \sum_{f\in V(\Phi)} x^{d_{df}^3}$$
$$DH(\Phi,x) = \sum_{fg\in E(\Phi)} x^{[d_{df}+d_{dg}]^2}, \qquad DF^*(\Phi,x) = \sum_{fg\in E(\Phi)} x^{(d_{df}^2+d_{dg}^2)}$$

Where d_{df} is the domination degree of the vertex $f \in V(\Phi)$ which is defined as:

Definition 1.1 ([34]). *For any vertex $f \in V(\Phi)$, the domination degree denoted by d_{df} and defined as the number of minimal dominating sets of Φ which contains f.*

For more details of domination topological indices and their applications see ([15–18]).

Observation 1.2 ([34]). $1 \leq d_{df} \leq \Upsilon_m(\Phi)$, *where $\Upsilon_m(\Phi)$ is denoted to the total number of minimal domination sets of Φ.*

Definition 1.3 ([34]). *The graph Φ is called $r-$domination regular graph if and only if $d_{df} = k$ for all $f \in V(\Phi)$.*

We can list some major of topological indices such as degree- based-topological indices and distance based-topological indices see [11–13]. For more discussion, see [1,3–8,10,29,35–37].

2. Second Domination Hyper Polynomial of Some Graph families

Definition 2.1. *For a connected simple graph Φ, the second domination hyper polynomial is define as:*

$$D_H Z_2(\Phi,x) = \sum_{fg\in E(\Phi)} x^{(d_{pf}d_{pg})^2} = \sum_{fg\in E(\Phi)} x^{d_{pf}^2 d_{pg}^2}.$$

Lemma 2.2 ([34]). *$\Upsilon_m(S_{r+1}) = 2$ and $\Upsilon_m(K_n) = n$. And for all $f \in V(S_{r+1})$ or $f \in V(K_n)$ we get $d_{df} = 1$.*

Proposition 2.3.

(1) In the star graph S_{r+1}

$$D_H Z_2(S_{r+1}, x) = rx$$

(2) For K_n, we have

$$D_H Z_2(K_n, x) = \frac{n(n-1)\, x}{2}$$

(3) For $S_{r+1,s+1}$, with $s+r+2$ vertices we have

$$D_H Z_2(S_{r+1,s+1}, x) = (r+s+1)x^{16}$$

Lemma 2.4 ([34]). $\Upsilon_m(K_{i,j}) = rs + 2$, *with* $i \geq 2$, $j \geq 2$ *and* $d_{df} = \begin{cases} i+1 \\ j+1 \end{cases}$ *for all* $f \in V(K_{i,j})$

Theorem 2.5. *If $\Phi \cong K_{i,j}$, with $i \geq 2$, $j \geq 2$ then*

$$D_H Z_2(\Phi, x) = rs\ x^{i^2j^2+2i^2j+i^2+2ij^2+4ij+2i+j^2+2j+1}.$$

Proof. Using lemma 2.4, we get

$$\begin{aligned} D_H Z_2(\Phi, x) &= \sum_{fg\in E(\Phi)} x^{d_{df}^2 d_{dg}^2} = \sum_{fg\in E(\Phi)} x^{(i+1)^2(j+1)^2} \\ &= \sum_{fg\in E(\Phi)} x^{(i^2+2i+1)(j^2+2j+1)} \\ &= \sum_{fg\in E(\Phi)} x^{(i^2j^2+2i^2j+i^2+2ij^2+4ij+2i+j^2+2j+1)} \\ &= rs\ x^{i^2j^2+2i^2j+i^2+2ij^2+4ij+2i+j^2+2j+1} \end{aligned}$$

□

One can define a Windmill graph $Wd_{r_1}^{r_2}$ as a graph obtained by taking r_2 copies of the complete graph K_{r_1} with a common vertex.

Lemma 2.6 ([34]). *Suppose Φ is $Wd_{r_1}^{r_2}$. Then $\Upsilon_m(Wd_{r_1}^{r_2}) = (r_1-1)^{r_2}+1$ and* $d_{df} = \begin{cases} 1, & \text{if } f \text{ is the center vertex;} \\ (r_1-1)^{r_2-1}, & \text{otherwise.} \end{cases}$

Theorem 2.7. *Let Φ be the Windmill graph $Wd_{r_1}^{r_2}$, then*

$$D_H Z_2(\Phi, x) = r_2(r_1-1)x^{(r_1-1)^{2(r_2-1)}} + \left(\frac{r_2(r_1-1)^2-(r_1-1)}{2}\right) x^{(r_1-1)^{4(r_2-1)}}.$$

Proof. Let w be the center vertex. Then the set edge of $Wd_{r_1}^{r_2}$ can be divided with respect to the domination degree as $E_1 = \{fw \in E(Wd_{r_1}^{r_2}) : w \text{ is the center vertex}\}$; $E_2 = \{fg \in E(K_{r_1}) : \{f,g\} \in V(K_{r_1})\}$, hence

$$\begin{aligned} D_H Z_2(\Phi, x) &= \sum_{fg\in E(\Phi)} x^{d_{df}^2 d_{dg}^2} = \sum_{fg\in E_1} x^{d_{df}^2 d_{dg}^2} + \sum_{fg\in E_2} x^{d_{df}^2 d_{dg}^2} \\ &= \sum_{fg\in E_1} x^{1^2\times(r_1-1)^{2(r_2-1)}} + \sum_{fg\in E_2} x^{(r_1-1)^{2(r_2-1)}\times(r_1-1)^{2(r_2-1)}} \end{aligned}$$

$$= x^{(r_1-1)^{2(r_2-1)}}|E_1| + x^{(r_1-1)^{2(r_2-1)}\times(r_1-1)^{2(r_2-1)}}|E_2|$$
$$= r_2(r_1-1)x^{(r_1-1)^{2(r_2-1)}} + \left(\frac{r_2(r_1-1)^2-(r_1-1)}{2}\right) x^{(r_1-1)^{4(r_2-1)}}.$$

□

Proposition 2.8. *Suppose Φ is $r-$domination-regular graph, then $D_HZ_2(\Phi,x) = x^{r^4}|E(\Phi)|$.*

Definition 2.9. *For any graphs Φ_1 and Φ_2 their cartesian product $G\times H$ is defined as [26] the graph on the vertex set $V(\Phi_1)\times V(\Phi_2)$ with vertices $f=(f_1,f_2)$ and $g=(g_1,g_2)$ are adjacent by an edge if and only if either $([f_1=g_1$ and $\{f_2,g_2\}\in E(\Phi_2)])$ or $([f_2=g_2$ and $\{f_1,g_1\}\in E(\Phi_1)])$.*

Definition 2.10 ([33]). *The book graph b_j is a cartesian product of a star S_{j+1} and single edge P_2 see Figure 1.*

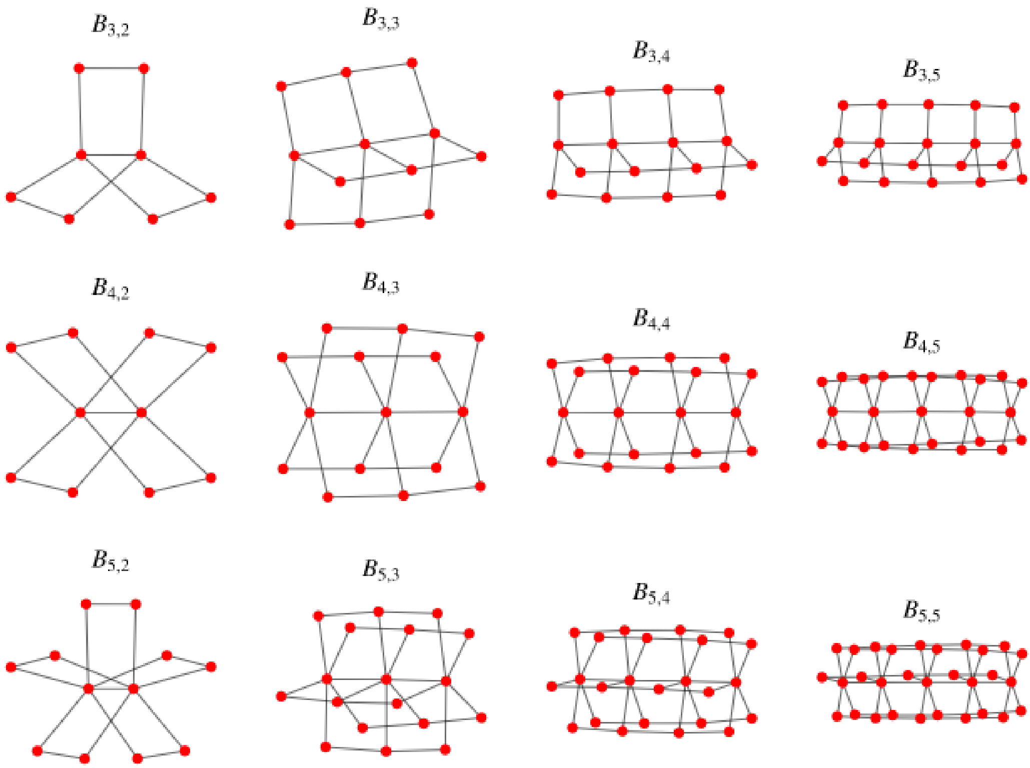

Figure 1: Book graph and stacked book graph

Lemma 2.11 ([34]). *Suppose $\Phi\cong b_j$, with $j\geq 3$. Then $\Upsilon_m(\Phi)=2^j+3$ and for $f\in V(b_j)$, we have:*

$$d_{df} = \begin{cases} 3, & \text{if } f \text{ is the center vertex;} \\ 2^{j-1}+1, & \text{otherwise.} \end{cases}$$

Theorem 2.12. $D_HZ_2(b_j,x) = j\,x^{\left(2^{(j-1)}+1\right)^4} + x^{\left(9(2^{(j-1)}+1)^2\right)} + x^{81}$.

Proof. One can partition the edges of book graph b_j as in Table 1.

$E_i = (d_{df}, d_{dg})$	Number of edges
$E_1 = (2^{j-1}+1, 2^{j-1}+1)$	j
$E_2 = (3,3)$	1
$E_3 = (3, 2^{j-1}+1)$	2j

Table 1: Edge partition of book graph

$$\begin{aligned}
D_H Z_2(bj,x) &= \sum_{fg\in E(bj)} x^{d_{df}^2 d_{dg}^2} \\
&= \sum_{fg\in E_1} x^{d_{df}^2 d_{dg}^2} + \sum_{fg\in E_2} x^{d_{df}^2 d_{dg}^2} + \sum_{fg\in E_3} x^{d_{df}^2 d_{dg}^2} \\
&= \sum_{fg\in E_1} x^{(2^{j-1}+1)^2\times(2^{j-1}+1)^2} + \sum_{fg\in E_2} x^{3^2\times 3^2} + \sum_{fg\in E_3} x^{3^2\times(2^{j-1}+1)^2} \\
&= x^{(2^{j-1}+1)^4}|E_1| + x^{81}|E_2| + x^{9(2^{j-1}+1)^2}|E_3| \\
&= j\; x^{\left(2^{(j-1)}+1\right)^4} + x^{\left(9(2^{(j-1)}+1)^2\right)} + x^{81}.
\end{aligned}$$

□

Lemma 2.13 ([34]). *Let Φ be any connected graph with order n_1 and size m_1. Let $H \cong \Phi \circ K_{n_2}$. There are $(n_2+1)^{n_1}$ minimal domination sets in H, and $d_{df} = (n_2+1)^{n_1-1}$.*

Theorem 2.14. *Let Φ be a graph with order n_1 and size m_1. Let K_{n_2} be a complete graph. Then*

$$D_H Z_2(\Phi\circ K_{n_2}, x) = x^{(n_2+1)^{4(n_1-1)}}|E(\Phi)| + \frac{n_1 n_2(n_2-1)}{2}\; x^{(n_2+1)^{4(n_1-1)}} + n_1 n_2 x^{(n_2+1)^{4(n_1-1)}}.$$

Proof. Note that the order of $(\Phi\circ K_{n_2})$ *is* $n_1 + n_1 n_2$ and $G\circ K_{n_2}$ is $(n_2+1)^{n_1-1}$ domination regular graph. Also, based on domination degree of the vertices of $\Phi\circ K_{n_2}$, one can divided the edges of $\Phi\circ K_{n_2}$ as

$$\begin{aligned}
E_1 &= \{fg \in E(\Phi\circ K_{n_2}) : fg \in E(\Phi)\} \\
E_2 &= \{fg \in E(\Phi\circ K_{n_2}) : fg \in E(K_{n_2})\} \\
E_3 &= \{uv \in E(\Phi\circ K_{n_2}) : f \in V(\Phi), g \in V(K_{n_2})\}
\end{aligned}$$

Hence,

$$\begin{aligned}
D_H Z_2(\Phi\circ K_{n_2}, x) &= \sum_{fg\in E(\Phi\circ K_{n_2})} x^{d^2_{df\Phi\circ K_{n_2}} d^2_{dg\Phi\circ K_{n_2}}} \\
&= \sum_{fg\in E_1} x^{d^2_{df\Phi\circ K_{n_2}} d^2_{dg\Phi\circ K_{n_2}}} + \sum_{fg\in E_2} x^{d^2_{df\Phi\circ K_{n_2}} d^2_{dg\Phi\circ K_{n_2}}} + \sum_{fg\in E_3} x^{d^2_{df\Phi\circ K_{n_2}} d^2_{dg\Phi\circ K_{n_2}}} \\
&= \sum_{fg\in E_1} x^{(n_2+1)^{2(n_1-1)}\times(n_2+1)^{2(n_1-1)}}
\end{aligned}$$

$$+ \sum_{fg\in E_2} x^{(n_2+1)^{2(n_1-1)}\times(n_2+1)^{2(n_1-1)}} + \sum_{fg\in E_3} x^{(n_2+1)^{2(n_1-1)}\times(n_2+1)^{2(n_1-1)}}$$
$$= x^{(n_2+1)^{4(n_1-1)}}|E_1| + x^{(n_2+1)^{2(n_1-1)}}|E_2| + x^{(n_2+1)^{2(n_1-1)}}|E_3|$$
$$= x^{(n_2+1)^{4(n_1-1)}}|E(\Phi)| + \frac{n_1n_2(n_2-1)}{2}\ x^{(n_2+1)^{4(n_1-1)}} + n_1n_2x^{(n_2+1)^{4(n_1-1)}}.$$

□

Lemma 2.15 ([34]). *Suppose $H \cong \Phi \circ \overline{K_{n_2}}$ where Φ be a graph of order n_1. Then $\Upsilon_m(H) = \sum_{i=0}^{n_1} \binom{n_1}{i}$.*

Theorem 2.16. *Suppose Φ is a graph of order n_1 and size m_1.*

$$D_HZ_2(\Phi\circ\overline{K_{n_2}},x) = x^{\left(\Upsilon_m(\Phi\circ\overline{K_{n_2}})\right)^4}|E(\Phi\circ\overline{K_{n_2}})|.$$

Proof. Any every $f \in V(\Phi\circ\overline{K_{n_2}})$ is contained in every minimal dominating sets of $\Phi\circ\overline{K_{n_2}}$ except $\binom{n_1-1}{0} + \binom{n_1-1}{1} + ... + \binom{n_1-1}{n_1-2} + \binom{n_1-1}{n_1-1} = 2^{n_1-1}$ minimal dominating sets. Hence, $d_{df\Phi\circ\overline{K_{n_2}}} = \Upsilon_m(\Phi\circ\overline{K_{n_2}}) - 2^{n_1-1}$ and by using the definition of second domination hyper index we get:

$$D_HZ_2(\Phi\circ\overline{K_{n_2}},x) = \sum_{fg\in E(\Phi\circ\overline{K_{n_2}})} x^{d_{df}^2 d_{dg}^2}$$
$$= \sum_{fg\in E(\Phi\circ\overline{K_{n_2}})} x^{\left(\Upsilon_m(\Phi\circ\overline{K_{n_2}})-2^{n_1-1}\right)^2\times\left(\Upsilon_m(\Phi\circ\overline{K_{n_2}})-2^{n_1-1}\right)^2}$$
$$= \sum_{fg\in E(\Phi\circ\overline{K_{n_2}})} x^{\left(\Upsilon_m(\Phi\circ\overline{K_{n_2}})-2^{n_1-1}\right)^4}$$
$$= x^{\left(\Upsilon_m(\Phi\circ\overline{K_{n_2}})\right)^4}|E(\Phi\circ\overline{K_{n_2}})|.$$

□

3. Second Domination Hyper Polynomial of Hexane Isomers

The properties that characterize the different chemical compounds are closely related to the molecular structure of these compounds. In this section, we calculate the second domination polynomial of Hexane isomers. Hexane C_6H_{14} is an alkane hydrocarbon compound, the first part "hex" means the six carbon atoms, while the second part "ane" means that the carbon atoms are linked by single chemical bonds. Hexane isomers are often used as inert solvents in many organic chemical reactions because they are non-polar compounds. They can also be considered components of gasoline and adhesives that can be used in footwear or leather products. Hexane can also be used in solvents for the purpose of extracting oils for cooking, and in the laboratory, it can be used to extract grease and oils from water or soil. Hexane has four isomers: Hexane, 2-methylpentane, 2, 2-dimethylbutane, and 2, 3-dimethybutane. In this study, we include hexane isomers (see Fig 2, 3).

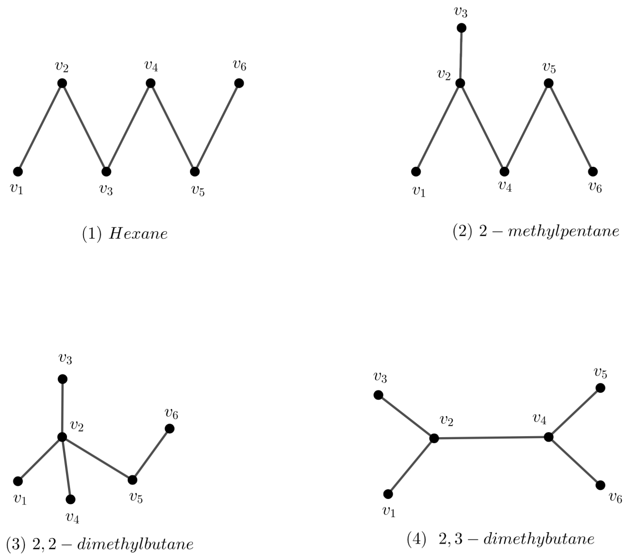

Figure 2: Molecular graph of hexane isomers.

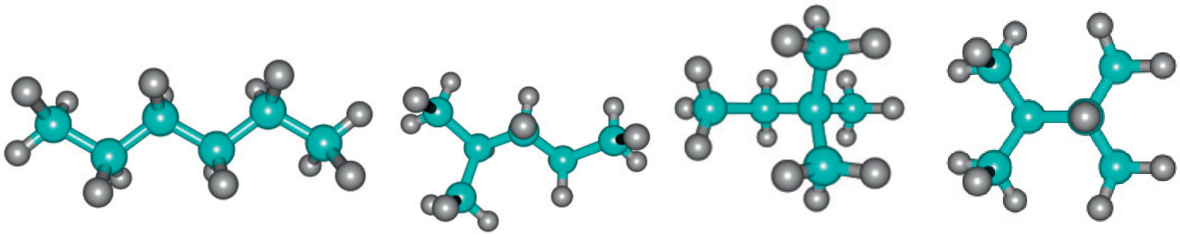

Figure 3: Chemical structures of hexane isomers.

Theorem 3.1. *If G_1 is the molecular graph of hexane, then $D_HZ_2(G_1, x) = 2x^{81} + x^{64} + x^{36} + x^{16}$.*

Proof. If G_1 is the molecular graph of hexane, by using the definition of domination degree we get, $d_d(v_1) = 4$, $d_d(v_2) = d_d(v_3) = 2$, $d_d(v_4) = d_d(v_5) = d_d(v_6) = 3$, hence

$$\begin{aligned} D_HZ_2(G_1, x) &= \sum_{fg \in E(G_1)} x^{(d_{df} d_{dg})^2} = x^{(4\times2)^2} + x^{(2\times2)^2} + x^{(2\times3)^2} + 2x^{(3\times3)^2} \\ &= 2x^{81} + x^{64} + x^{36} + x^{16}. \end{aligned}$$

□

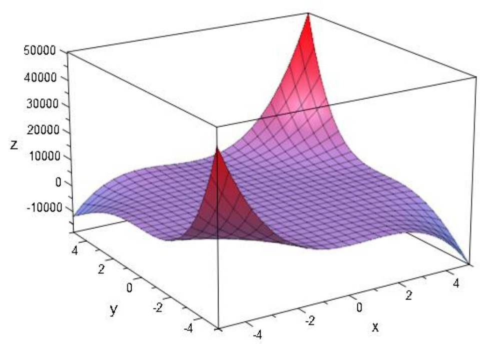

Figure 4: Plotting of second domination hyper polynomial of Hexane.

Theorem 3.2. *Suppose G_2 is the molecular graph of 2-methylpentane, then* $D_H Z_2(G_2, x) = x^{81} + 2x^{36} + x^9 + x^4$.

Proof. Suppose G_2 is the molecular graph of 2-methylpentane, then applying the definition of domination degree one can get the following: $d_d(v_1) = d_d(v_2) = d_d(v_6) = 3$, $d_d(v_3) = d_d(v_5) = 2$, $d_d(v_4) = 1$, hence

$$D_H Z_2(G_2, x) = \sum_{fg \in E(G_2)} x^{(d_{d_f} d_{d_g})^2} = x^{(3\times3)^2} + 2x^{(3\times2)^2} + x^{(3\times1)^2} + x^{(2\times1)^2}$$
$$= x^{81} + 2x^{36} + x^9 + x^4.$$

□

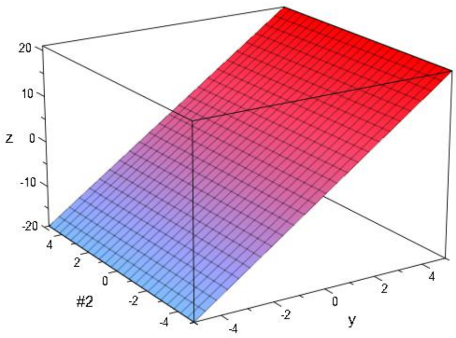

Figure 5: Plotting of second domination hyper polynomial of 2-methylpentane.

Theorem 3.3. *Suppose G_3 is the molecular graph of 2, 2-dimethylbutane, then,* $D_H Z_2(G_3, x) = 5x^{16}$.

Proof. Let G_3 be the molecular graph of 2, 2-dimethylbutane. Applying the definition of domination degree one can get the following: $d_d(v) = 2$ for all $v \in G_3$. Hence

$$D_H Z_2(G_3, x) = \sum_{fg \in E(G_3)} x^{(d_{d_f} d_{d_g})^2} = x^{(2\times2)^2} + x^{(2\times2)^2} + x^{(2\times2)^2} + x^{(2\times2)^2} + +x^{(2\times2)^2}$$
$$= 5x^{16}.$$

□

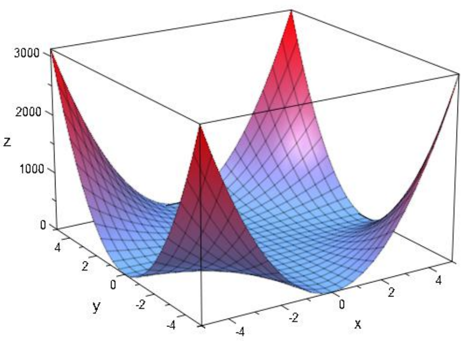

Figure 6: Plotting of second domination hyper polynomial of 2, 2-dimethylbutane.

Theorem 3.4. *Let G_4 be the molecular graph of 2, 3-dimethybutane. Then, $D_HZ_2(G_4, x) = 5x^{16}$.*

Proof. Let G_4 be the molecular graph of 2, 3-dimethybutane. Applying the definition of domination degree one can get the following: $d_d(v) = 2$ for all $v \in G_4$. Hence

$$D_HZ_2(G_4, x) = \sum_{fg \in E(G_4)} x^{(d_{df} d_{dg})^2} = x^{(2\times2)^2} + x^{(2\times2)^2} + x^{(2\times2)^2} + x^{(2\times2)^2} + +x^{(2\times2)^2}$$
$$= 5x^{16}.$$

□

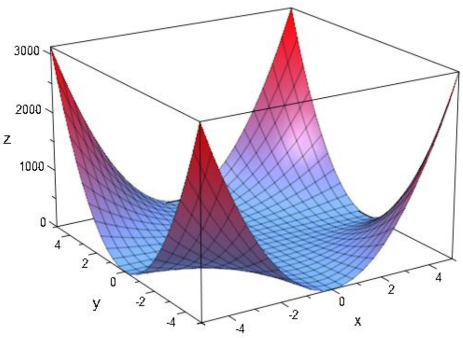

Figure 7: Plotting of second domination hyper polynomial of 2, 3-dimethybutane.

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