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Computation Domination and γ −Domination Topological Indices of Hexane Isomers via φ_P −Polynomial with QSPR Analysis

Hanan Ahmed [1,*], Rangarajan Raghavachar [2], Abdu Alameri [3], Ruby Salestina Morgan [1]

[1] Department of Mathematics, Yuvarajas College, University of Mysore, Mysuru, India; hananahmed1a@gmail.com (H.A); ruby.salestina@gmail.com (R.S);
[2] Department of Studies in Mathematics, Manasagangotri, University of Mysore, Mysuru, India; ajra63@gmail.com (R.R.);
[3] Department of Biomedical Engineering, Faculty of Engineering, University of Science and Technology, Yemen; a.alameri2222@gmail.com (A.A.);
* Correspondence: hananahmed1a@gmail.com (H.A.);

Scopus Author ID 57222051555
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Abstract: The properties that characterize the different chemical compounds are closely related to the molecular structure of these compounds. A topological index is a number or numerical quantity derived from the graph of a chemical compound. It is used to model compounds' physical and chemical properties and activities, such as hexane isomers. It was presented new topological indices known as the domination and $\gamma -$ domination topological indices. In this paper, we study the importance and applications of these indicators in determining some physical and chemical properties of hexane isomers. Moreover, the $\varphi_P -$ polynomial is used in calculating these indices.

Keywords: Domination and γ-domination topological indices; domination degree; domination value; hexane isomers.

1. Introduction

Chemical graph theory is one of the branches of mathematical chemistry, as it is important and necessary for a better understanding and explanation of the nature of the chemical structure. By International Union of Pure and Applied Chemistry (IUPAC) terminology, a topological index is a numerical value correlation of chemical structure with different physical and chemical properties. In exact phrase, topological indices are numerical parameters of the graph, such that these parameters are the same for the graph, which are isomorphism. A molecular graph [1, 2] is a simple connected graph such that the vertices and edges are supposed to be atoms and chemical bonds, respectively. Chemical graph theory is an important branch of both chemistry and graph theory. It has taken a lot of attention because of the important results obtained in chemical graph theory and has been applied in many applications such as chemical engineering and pharmaceutical. The main idea of chemical graph theory is that molecules' physical and chemical properties can be studied and explained using information. It can also be noted that in the contemporary mathematical and chemical literature, there are many descriptors of molecular structure based on vertex degree. Let $G = (V(G), E(G))$ be a finite simple connected graph consisting of a set of objects $V(G)$ called vertices, and another set $E(G)$ whose elements are called edges. A set $D \subseteq V$ is said to be a

dominating set of graph G if, for any vertex $v \in V - D$, there exists a vertex $u \in D$ such that u and v are adjacent. A dominating-set $D = \{v_1, v_2, \ldots, v_r\}$ is minimal if $D - v_i$ is not a dominating set [3], a dominating set of G of minimum cardinality is said to be a minimum dominating set. For specifics on domination in graphs, see [4-6]. Hanan Ahmed et al. [7-9] presented novel topological indices known as the domination and $\gamma -$ domination topological indices. The first and second domination Zagreb, forgotten domination, hyper domination indices are defined as:

$$DM_1(G) = \sum_{v \in V(G)} d_d^2(v), \quad DM_2(G) = \sum_{uv \in E(G)} d_d(u) d_d(v),$$

$$DM_1^*(G) = \sum_{uv \in E(G)} \left(d_d(u) + d_d(v)\right), \quad DF^*(G) = \sum_{uv \in E(G)} \left(d_d^2(u) + d_d^2(v)\right),$$

$$DF(G) = \sum_{v \in V(G)} d_d^3(v), \quad DH(G) = \sum_{uv \in E(G)} (d_d(u) + d_d(v))^2.$$

where $d_d(v)$ is the domination degree of $v \in V(G)$ and defined as the number of minimal dominating sets of G which contains v. The $\gamma -$domination Zagreb, $\gamma -$domination forgotten, $\gamma -$domination hyper indices are defined as:

$$\gamma M_1(G) = \sum_{v \in V(G)} d_\gamma^2(v), \quad \gamma M_2(G) = \sum_{uv \in E(G)} d_\gamma(u) d_\gamma(v),$$

$$\gamma F(G) = \sum_{v \in V(G)} d_\gamma^3(v), \quad \gamma H(G) = \sum_{uv \in E(G)} (d_\gamma(u) + d_\gamma(v))^2,$$

$$\gamma M_1^*(G) = \sum_{uv \in E(G)} \left(d_\gamma(u) + d_\gamma(v)\right), \quad \gamma F^*(G) = \sum_{uv \in E(G)} \left(d_\gamma^2(u) + d_\gamma^2(v)\right).$$

where $d_\gamma(v)$ is the domination value of v and defined as the number of minimum dominating sets of G which contains v. More recent outcomes of topological indices and their applications are reported in [10-25].

Definition 1.1.

Let $G = (V, E)$ be a graph, $d_P(v)$ be the P set degree of the vertex v denoted by:

$$d_P(v) = |\{Q \subseteq V(G): Q \ \ has \ \ property \ \ P \ \ and \ \ v \in Q\}|.$$

The minimum and maximum P set degree of G denoted as $\delta_P(G) = \delta_P$ and $\Delta_P(G) = \Delta_P$ respectively. Such that $\delta_P = min\{d_P(v): v \in V(G)\}$ and $\Delta_P = max\{d_P(v): v \in V(G)\}$.

Let $d_P m_{i,j}(G) = |\{e = uv: d_P(u) = i, d_P(v) = j\}|$. The φ_P-polynomial is defined as:

$$\varphi_P(G, x, y) = \sum_{\delta_P \le i \le j \le \Delta_P} d_P m_{i,j}(G) x^i y^j .$$

Table 1. The description of some domination and γ −domination topological indices.

D indices	$\mathbf{f(d_d(u), d_d(v))}$	**γD indices**	$\mathbf{f(d_\gamma(u), d_\gamma(v))}$
$DM_1^*(G)$	$d_d(u) + d_d(v)$	$\gamma M_1^*(G)$	$d_\gamma(u) + d_\gamma(v)$
$DF^*(G)$	$d_d^2(u) + d_d^2(v)$	$\gamma F^*(G)$	$d_\gamma^2(u) + d_\gamma^2(v)$
$DM_2(G)$	$d_d(u) + d_d(v)$	$\gamma M_2(G)$	$d_\gamma(u) d_\gamma(v)$
$HD(G)$	$d_d^2(u) + d_d^2(v) + 2d_d(u) d_d(v)$	$\gamma H(G)$	$d_\gamma^2(u) + d_\gamma^2(v) + 2d_\gamma(u) d_\gamma(v)$

Domination (D) and γ −Domination (γD) indices defined on E(G) can be written as in Table1 and:

$$\mathrm{D(G)} = \sum_{\mathrm{uv \in E(G)}} \mathrm{f\left(d_d(u), d_d(v)\right)}, \quad \mathrm{\gamma D(G)} = \sum_{\mathrm{uv \in E(G)}} \mathrm{f\left(d_\gamma(u), d_\gamma(v)\right)}.$$

Table 2. Derivation of domination and γ −domination topological indices from φ_P −polynomials.

D indices	Derivation from $\boldsymbol{\varphi_d(G)}$	γD indices	Derivation from $\boldsymbol{\varphi_\gamma(G)}$
$DM_1^*(G)$	$(D_x + D_y)(\varphi_d(G))\|_{x=y=1}$	$\gamma M_1^*(G)$	$(D_x + D_y)(\varphi_\gamma(G))\|_{x=y=1}$
$DF^*(G)$	$(D_x^2 + D_y^2)(\varphi_d(G))\|_{x=y=1}$	$\gamma F^*(G)$	$(D_x^2 + D_y^2)(\varphi_\gamma(G))\|_{x=y=1}$
$DM_2(G)$	$(D_xD_y)(\varphi_d(G))\|_{x=y=1}$	$\gamma M_2(G)$	$(D_xD_y)(\varphi_\gamma(G))\|_{x=y=1}$
$HD(G)$	$(D_x + D_y)^2(\varphi_d(G))\|_{x=y=1}$	$\gamma H(G)$	$(D_x + D_y)^2(\varphi_\gamma(G))\|_{x=y=1}$

Here $D_x(f(x,y)) = x\frac{\partial(f(x,y))}{\partial x}$, $D_y(f(x,y)) = y\frac{\partial(f(x,y))}{\partial y}$.

2. Materials and Methods

The main results acquired in this article are based on domination and γ- domination topological indices of hexane isomers with the help of φ_P-polynomials. In the diagram (Figure 1), we consider only the vertices, which are not hydrogen atoms, as a hydrogen atom does not produce any contribution. We have used an edge segmentation method, analytical methods, and the score-counting method to draw conclusions. We have computed all minimal dominating sets and minimum dominating sets, and with these sets, we have computed the domination degree and the domination value for all vertices of the graph. We also divided the edges based on the new degrees and calculated φ_P-polynomials, since through these φ_P-polynomials we can get domination and γ-domination indices with the help of Table 2. We use R software for calculating the linear regression analysis.

3. Results and Discussion

3.1. Domination and $\boldsymbol{\gamma}$ −domination indices 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 single chemical bonds link the carbon atoms. Hexane isomers are often used as inert solvents in many organic chemical reactions because they are non-polar compounds.

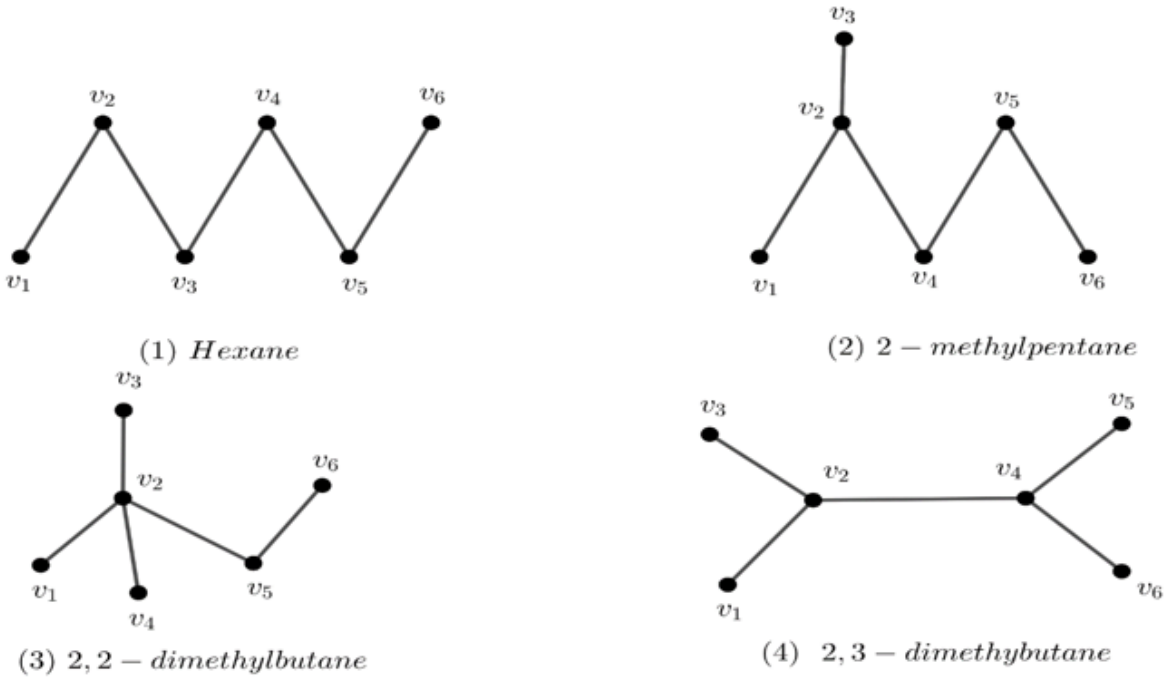

Figure 1. Molecular graph of hexane isomers except for 3-methylpentane.

They can also be considered as 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. In this section, we will calculate the exact values of the domination topological indices using φ_P −polynomial. Hexane has five isomers: Hexane, 2-methylpentane, 3-methylpentane, 2, 2-dimethylbutane, and 2, 3-dimethybutane.

In this study, we include hexane isomers except for 3-methylpentane (Figures 1, 2). The 3-methylpentane isomer was excluded because of the extreme values of the topological indices in this isomer.

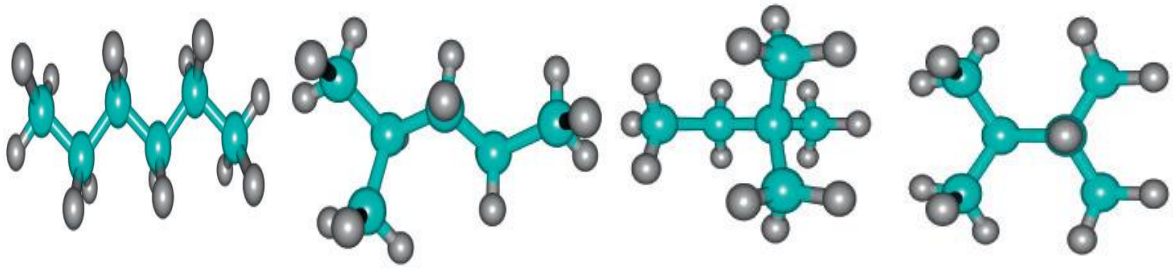

Figure 2. Chemical structures of hexane isomers except for 3-methylpentane.

Theorem 3.1.1.

Let G_1 be the molecular graph of hexane. Then:

$$\varphi_d(G_1, x, y) = x^2(y^4 + y^2 + y^3) + 2x^3y^3,$$

$$\varphi_\gamma(G_1, x, y) = 4y + 1.$$

Proof. If G_1 is the molecular graph of hexane; note that the total number of minimal dominating sets of G_1 are six minimal dominating sets. Among them, there is only one minimum dominating set $D = \{v_2, v_5\}$. Hence by using the definition of domination degree and domination value, we get, $d_d(v_1) = 4, d_d(v_2) = d_d(v_3) = 2, d_d(v_4) = d_d(v_5) = d_d(v_6) = 3$, and $d_\gamma(v_1) = d_\gamma(v_3) = d_\gamma(v_4) = d_\gamma(v_6) = 0, d_\gamma(v_2) = d_\gamma(v_5) = 1$. And the partition of edges of G_1 depends on domination degree and domination value are given in Table 3.

Table 3. Edge partitions.

$d_d m_{ij}$	(2,4)	(2,2)	(2,3)	(3,3)
No. of edges	1	1	1	2
$d_\gamma m_{ij}$	(0,1)	(0,0)		
No. of edges	4	1		

Then:

$$\varphi_d(G_1, x, y) = \sum_{\delta_d \le i \le j \le \Delta_d} d_d m_{i,j}(G_1) x^i y^j$$

$$= x^2(y^4 + y^2 + y^3) + 2x^3y^3,$$

$$\varphi_\gamma(G_1, x, y) = \sum_{\delta_\gamma \le i \le j \le \Delta_\gamma} d_\gamma m_{i,j}(G_1) x^i y^j$$

$$= 4y + 1.$$

In Figure 3, we plot of φ_d −polynomial and φ_γ −polynomial of hexane.

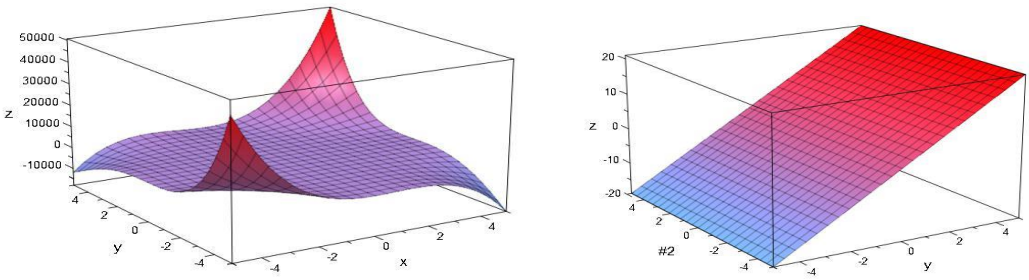

Figure 3. Plotting of (a)φ_d −polynomial and (b) φ_γ −polynomial of hexane.

Proposition 3.1.2.

Suppose G_1 is the molecular graph of hexane, then:

$$DM_1^*(G_1) = 27, \quad \gamma M_1^*(G_1) = 4, \quad DM_2(G_1) = 36, \quad \gamma M_2(G_1) = 0,$$

$$DF^*(G_1) = 77, \quad \gamma F^*(G_1) = 4, \quad DH(G_1) = 149, \quad \gamma H(G_1) = 4,$$

$$DM_1(G_1) = 51, \quad \gamma(G_1) = 2, \quad DF(G_1) = 161, \quad \gamma F(G_1) = 2.$$

Proof. We have:

$$\varphi_d(G_1, x, y) = x^2(y^4 + y^2 + y^3) + 2x^3y^3,$$

$$\varphi_\gamma(G_1, x, y) = 4y + 1.$$

Using Table 2, we have:

$$DM_1^*(G_1) = x^2(6y^4 + 4y^2 + 5y^3) + 12x^3y^3|_{x=y=1} = 27,$$

$$DM_2(G_1) = 2x^2(4y^4 + 2y^2 + 3y^3) + 18x^3y^3|_{x=y=1} = 36,$$

$$DF^*(G_1) = x^2(20y^4 + 8y^4 + 13y^3) + 36x^3y^3|_{x=y=1} = 77,$$

$$DH(G_1) = x^2(36y^4 + 16y^2 + 25y^3) + 72x^3y^3|_{x=y=1} = 149,$$

$$\gamma M_1^*(G_1) = 4y|_{x=y=1} = 4, \ \gamma M_2(G_1) = 0, \ \gamma F^*(G_1) = 4y|_{x=y=1} = 4,$$

$$\gamma H(G_1) = 4y|_{x=y=1} = 4.$$

By using the definition of $DM_1(G_1)$, $DF(G_1)$, $\gamma M_1(G_1)$ and $\gamma F(G_1)$ we get:

$$DM_1(G_1) = 51, \quad \gamma M_1(G_1) = 2, \quad DF(G_1) = 161, \quad \gamma F(G_1) = 2.$$

Theorem 3.1.3.

Suppose G_2 is the molecular graph of 2-methylpentane, then:

$$\varphi_d(G_2, x, y) = 2x^2y^3 + y^3(x^3 + x) + xy^2,$$

$$\varphi_\gamma(G_2, x, y) = 5y.$$

Proof. Let G_2 is the molecular graph of 2-methylpentane. It is easy to see that the total number of minimal dominating sets is five; among them, there is only one set $D = \{v_2, v_5\}$ which is minimum. Applying the definition of domination degree and domination value, one can get the following: $d_d(v_1) = d_d(v_2) = d_d(v_6) = 3$, $d_d(v_3) = d_d(v_5) = 2$, $d_d(v_4) = 1$,

and $d_\gamma(v_1) = d_\gamma(v_3) = d_\gamma(v_4) = d_\gamma(v_6) = 0, d_\gamma(v_2) = d_\gamma(v_5) = 1$. The partition of edges of G_2 depends on domination degree and domination value are given in Table 4.

Table 4. Edge partitions.

$d_d m_{ij}$	(2,3)	(3,3)	(1,3)	(1,2)
No. of edges	2	1	1	1
$d_\gamma m_{ij}$	(0,1)			
No. of edges	5			

Then:

$$\varphi_d(G_2, x, y) = \sum_{\delta_d \le i \le j \le \Delta_d} d_d m_{i,j}(G_2) x^i y^j$$

$$= 2x^2y^3 + y^3(x^3 + x) + xy^2,$$

$$\varphi_\gamma(G_2, x, y) = \sum_{\delta_\gamma \le i \le j \le \Delta_\gamma} d_\gamma m_{i,j}(G_2) x^i y^j$$

$$= 5y.$$

In Figure 4, we plot of φ_d −polynomial and φ_γ −polynomial of 2-methylpentane.

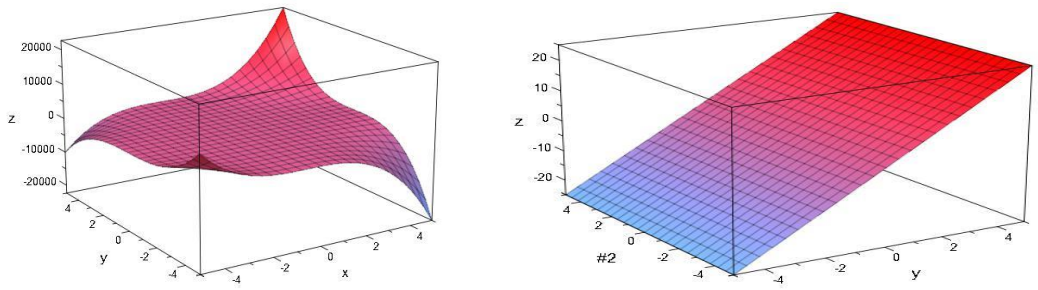

Figure 4. Plotting of (a)φ_d −polynomial and (b) φ_γ −polynomial of 2-methylpentane.

Proposition 3.1.4.

Suppose G_2 is the molecular graph of 2-methylpentane, then:

$$DM_1^*(G_2) = 23, \quad \gamma M_1^*(G_2) = 5, \quad DM_2(G_2) = 26, \quad \gamma M_2(G_2) = 0,$$

$$DF^*(G_2) = 59, \quad \gamma F^*(G_2) = 5, \quad DH(G_2) = 111, \quad \gamma H(G_2) = 5,$$

$$DM_1(G_2) = 36, \quad \gamma(G_2) = 2, \quad DF(G_2) = 98, \quad \gamma F(G_2) = 2.$$

Proof. We have:

$$\varphi_d(G_2, x, y) = 2x^2y^3 + y^3(x^3 + x) + xy^2,$$

$$\varphi_\gamma(G_2, x, y) = 5y.$$

Using Table 2, we get:

$$DM_1^*(G_2) = 10x^2y^3 + y^3(6x^3 + 4x) + 3xy^2|_{x=y=1} = 23,$$

$$DM_2(G_2) = 12x^2y^3 + 3y^3(3x^3 + x) + 2xy^2|_{x=y=1} = 26,$$

$$DF^*(G_2) = 26x^2y^3 + y^3(18x^3 + 10x) + 5xy^2|_{x=y=1} = 59,$$

$$DH(G_2) = 50x^2y^3 + y^3(36x^3 + 16x) + 9xy^2|_{x=y=1} = 111,$$

$$\gamma M_1^*(G_2) = 5y|_{x=y=1} = 5,\ \gamma M_2(G_2) = 0,\ \gamma F^*(G_2) = 5y|_{x=y=1} = 5,$$

$$\gamma H(G_2) = 5y|_{x=y=1} = 5.$$

By using the definition of $DM_1(G_2)$, $DF(G_2)$, $\gamma M_1(G_2)$ and $\gamma F(G_2)$ we get:

$$DM_1(G_2) = 36, \quad \gamma M_1(G_2) = 2, \quad DF(G_2) = 98, \quad \gamma F(G_2) = 2.$$

Theorem 3.1.5.

Suppose G_3 is the molecular graph of 2, 2-dimethylbutane, then:

$$\varphi_d(G_3, x, y) = 5x^2y^2,$$

$$\varphi_\gamma(G_3, x, y) = y^2(3 + x) + xy.$$

Proof. Suppose G_3 is the molecular graph of 2, 2-dimethylbutane. It is easy to see that the total number of minimal dominating sets is four. Among them, there are two minimum dominating sets $D_1 = \{v_2, v_5\}$, and $D_2 = \{v_2, v_6\}$. Applying the definition of domination degree and domination value, one can get the following: $d_d(v) = 2$ for all $v \in G_3$ and $d_\gamma(v_1) = d_\gamma(v_3) = d_\gamma(v_4) = 0$, $d_\gamma(v_2) = 2$, $d_\gamma(v_5) = d_\gamma(v_6) = 1$. The partition of edges of G_3 depends on domination degree and domination value are given in Table 5.

Table 5. Edge partitions.

$d_d m_{ij}$	(2,2)		
No. of edges	5		
$d_\gamma m_{ij}$	(0,2)	(1,2)	(1,1)
No. of edges	3	1	1

Then:

$$\varphi_d(G_3, x, y) = \sum_{\delta_d \le i \le j \le \Delta_d} d_d m_{i,j}(G_3) x^i y^j$$

$$= 5x^2y^2,$$

$$\varphi_\gamma(G_3, x, y) = \sum_{\delta_\gamma \le i \le j \le \Delta_\gamma} d_\gamma m_{i,j}(G_3) x^i y^j$$

$$= y^2(3 + x) + xy.$$

In Figure 5, we plot of φ_d −polynomial and φ_γ −polynomial of 2, 2-dimethylbutane.

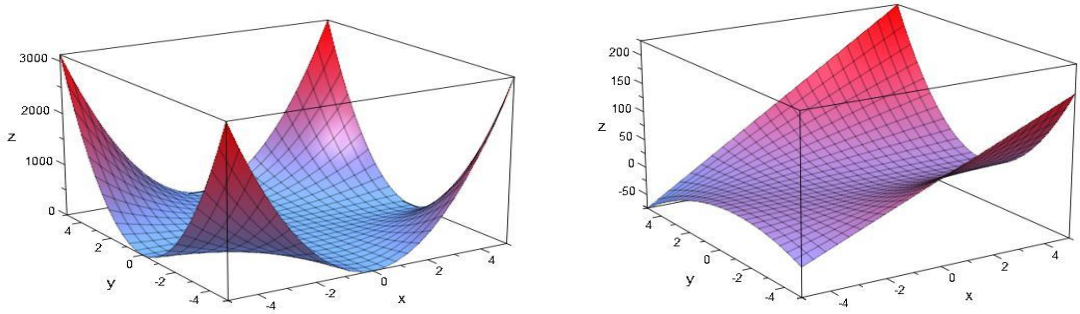

Figure 5. Plotting of (a)φ_d −polynomial and (b) φ_γ −polynomial of 2, 2-dimethylbutane.

By applying Theorem 3.1.5. and Table 2, one can prove the following Proposition.

Proposition 3.1.6.

Suppose G_3 is the molecular graph of 2, 2-dimethylbutane, then:

$$DM_1^*(G_3) = 20, \quad \gamma M_1^*(G_3) = 11, \quad DM_2(G_3) = 20, \quad \gamma M_2(G_3) = 3,$$

$$DF^*(G_3) = 40, \quad \gamma F^*(G_3) = 19, \quad DH(G_3) = 80, \quad \gamma H(G_3) = 25,$$

$$DM_1(G_3) = 24, \quad \gamma M_1(G_3) = 6, \quad DF(G_3) = 48, \quad \gamma F(G_3) = 10.$$

Using a similar way, one can prove the following Theorem and Proposition.

Theorem 3.1.7.

Let G_4 be the molecular graph of 2, 3-dimethybutane. Then:

$$\varphi_d(G_4, x, y) = 5x^2y^2,$$

$$\varphi_\gamma(G_4, x, y) = y(4 + x).$$

In Figure 6, we plot of φ_d −polynomial and φ_γ −polynomial of 2, 3-dimethybutane.

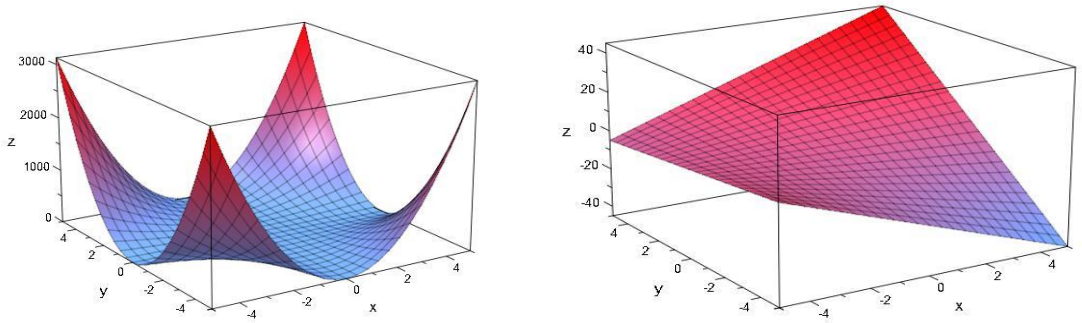

Figure 6. Plotting of (a)φ_d −polynomial and (b) φ_γ −polynomial of 2, 3-dimethybutane.

Proposition 3.1.8.

Suppose G_4 is the molecular graph of 2, 3-dimethybutane, then:

$$DM_1^*(G_4) = 20, \quad \gamma M_1^*(G_4) = 6, \quad DM_2(G_4) = 20, \quad \gamma M_2(G_4) = 1,$$

$$DF^*(G_4) = 40, \quad \gamma F^*(G_3) = 6, \quad DH(G_4) = 80, \quad \gamma H(G_4) = 8,$$

$$DM_1(G_4) = 24, \quad \gamma M_1(G_4) = 2, \quad DF(G_4) = 48, \quad \gamma F(G_4) = 2.$$

3.2. Motivation and application.

In this part, we will show the importance of domination of topological indices in determining the physicochemical properties in Table 7. In this study, we used the linear regression analysis modeled as $y = a + bx$, where y is the physicochemical properties of hexane isomers, and x represents the domination topological indices. These were calculated using R software for the values of four physicochemical properties and the twelve domination and γ −domination topological indices of hexane isomers. The exact values of domination and γ −domination topological indices were calculated by φ_P −polynomial of hexane isomers is given in Table 6.

Table 6. Domination and γ −domination topological indices of hexane isomers.

Hexane isomers	DM_1^*	DM_2	DF^*	DH	DM_1	DF	γM_1^*	γM_2	γF^*	γH	γM_1	γF
Hexane	27	36	77	149	51	161	4	0	4	4	2	2
2-methylpentane	23	26	59	111	36	98	5	0	5	5	2	2
2, 2-dimethylbutane	20	20	40	80	24	48	11	3	19	25	6	10
2, 3-dimethybutane	20	20	40	80	24	48	6	1	6	8	2	2

Table 7. Some physicochemical properties of hexane isomers.

Hexane isomers	FLI	SLI	$BP.F°$	E.C./eV
Hexan	222	140	155.7	-6448.22
2-methylpentane	168	94	140.5	-6448.21
2, 2-dimethylbutane	120	65	121.5	-6448.2
2,3-dimethybutane	130	72	136.4	-6448.15

By using the above model of linear regression analysis, we can get the different linear models for domination and γ −domination topological indices as follows:

1- Modified first domination Zagreb index

$$FLI = -152.27 + 13.87\, DM_1^*(G),$$

$$SLI = -135.3 + 10.13\, DM_1^*(G),$$

$$B.P = 52.5 + 3.8\, DM_1^*(G),$$

$$E.C = (-6.448e + 03) - (6.667e - 03)\, DM_1^*(G).$$

2- Second domination Zagreb index:

$$FLI = 4.9 + 6.1\, DM_2(G),$$

$$SLI = -21.1 + 4.46\, DM_2(G),$$

$$B.P = 95.77 + 1.67\, DM_2(G),$$

$$E.C = (-6.448e + 03) - (2.865e - 03)\, DM_2(G).$$

3- Modified forgotten domination index:

$$FLI = 20.37 + 2.58\, DF^*(G),$$

$$SLI = -8.4 + 1.87\, DF^*(G),$$

$$B.P = 100.1 + 0.7\, DF^*(G),$$

$$E.C = (-6.448e + 03) - (1.279e - 03)\, DF^*(G).$$

4- Hyper domination index:

$$FLI = 12.5 + 1.4\, DH(G),$$

$$SLI = -14.75 + 1.027\, DH(G),$$

$$B.P = 97.9 + 0.386\, DH(G),$$

$$E.C = (-6.448e + 03) - (6.797e - 04)\, DH(G).$$

5- First domination Zagreb index:

$$FLI = 38.76 + 3.59\, DM_1(G),$$

$$SLI = 4.34 + 2.6\, DM_1(G),$$

$$B.P = 105.13 + 0.98\, DM_1(G),$$

$$E.C = (-6.448e + 03) - (1.735e - 03)\, DM_1(G).$$

6- Forgotten domination index:

$$FLI = 83.8 + 0.858\, DF(G),$$

$$SLI = 37.17 + 0.62\, DF(G),$$

$$B.P = 117.54 + 0.23\, DF(G),$$

$$E.C = (-6.448e + 03) - (4.144e - 04)\, DF(G).$$

7- Modified first γ −domination Zagreb index:

$$FLI = 234.4 - 11.44\, \gamma M_1^*(G),$$

$$SLI = 145.3 - 8.08\, \gamma M_1^*(G),$$

$$B.P = 165.7 - 4.18\, \gamma M_1^*(G),$$

$$E.C = (-6.448e + 03) - (1.379e - 03)\, \gamma M_1^*(G).$$

8- Second γ −domination Zagreb index:

$$FLI = 185 - 25\, \gamma M_2(G),$$

$$SLI = 110.08 - 17.33\, \gamma M_2(G),$$

$$B.P = 147.39 - 8.8\, \gamma M_2(G),$$

$$E.C = (-6.448e + 03) - (5.000e - 03)\, \gamma M_2(G).$$

9- Modified forgotten γ −domination index:

$$FLI = 197.19 - 4.37\, \gamma F^*(G),$$

$$SLI = 118.79 - 3.06\, \gamma F^*(G),$$

$$B.P = 153.22 - 1.72\, \gamma F^*(G),$$

$$E.C = (-6.448e + 03) + (4.273e - 14)\, \gamma F^*(G).$$

10- Hyper γ −domination index:

$$FLI = 194.58 - 3.29\, \gamma H(G),$$

$$SLI = 116.89 - 2.299\, \gamma H(G),$$

$$B.P = 151.75 - 1.259\, \gamma H(G),$$

$$E.C = (-6.448e + 03) + (2.076e - 04)\, \gamma H(G).$$

11- First γ −domination Zagreb index:

$$FLI = 200 - 13.33\, \gamma M_1(G),$$

$$SLI = 120.5 - 9.25\, \gamma M_1(G),$$

$$B.P = 155.55 - 5.67\,\gamma M_1(G),$$

$$E.C = (-6.448e + 03) - (1.667e - 03)\gamma M_1(G).$$

12- Forgotten γ −domination index:

$$FLI = 186.667 - 6.667\,\gamma F(G),$$

$$SLI = 111.25 - 4.6\,\gamma F(G),$$

$$B.P = 149.87 - 2.8\,\gamma F(G),$$

$$E.C = (-6.448e + 03) - (8.333e - 04)\,\gamma F(G).$$

Now, we present the correlation coefficients of domination and γ −domination indices with physicochemical properties of hexane isomers listed in Table 8.

Table 8. Correlation coefficients.

	DM_1^*	DM_2	DF^*	DH	DM_1	DF	γM_1^*	γM_2	γF^*	γH	γM_1	γF
FLI	0.9959	0.994	0.993	0.996	0.996	0.996	-0.77	-0.76	-0.667	-0.699	-0.57	-0.577
SLI	0.994	0.996	0.983	0.991	0.992	0.992	-0.743	-0.724	-0.638	-0.667	-0.546	-0.546
BP	0.902	0.899	0.898	0.901	0.901	0.902	-0.925	-0.892	-0.866	-0.879	-0.807	-0.807
E.C	-0.71	-0.67	-0.73	-0.72	-0.72	-0.71	0.14	0.23	3.4e-12	0.067	-0.12	-0.12

From Table 8, we see: there is a very strong (+) correlation between ELI and DM_1^* and the same can be observed with DM_2, DF^* , DH, DM_1, and DF, and a strong (-) correlation between ELI with γM_1^*, γM_2, γF^*, γH, and moderate (-) with γM_1, γF (Figure 7). There is a very strong (+) correlation between SLI with DM_1^*, and the same can be observed with DM_2, DF^* , DH, DM_1 and DF. The correlation between SLI with γM_1^*, γM_2, γF^*, γH is strong(-) while, the correlation is moderate (-) γM_1 and γF (Figure 8).

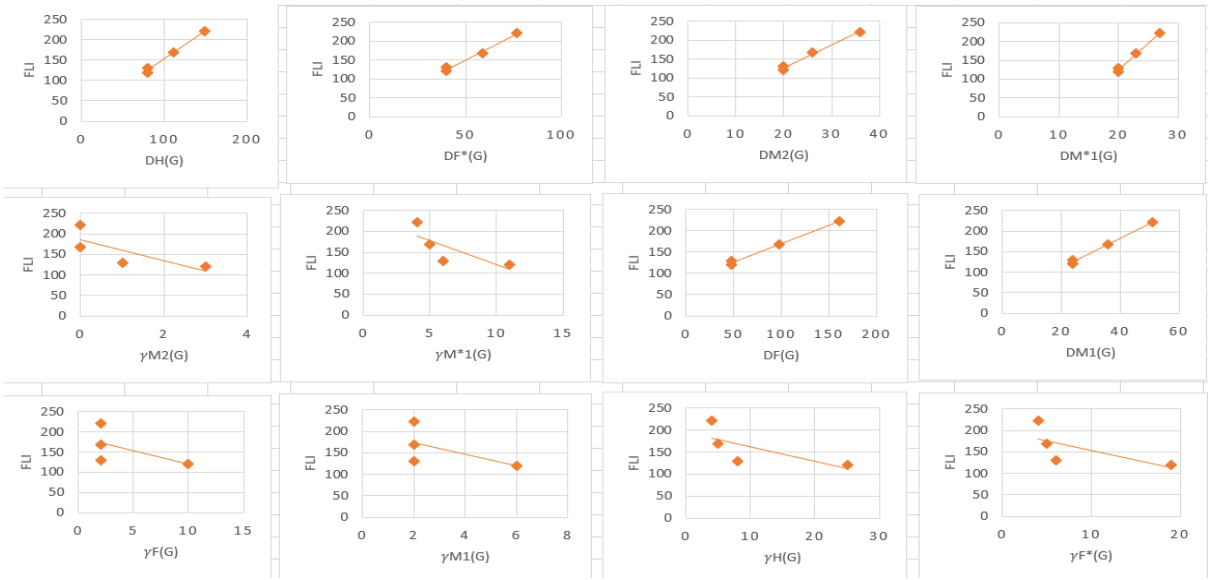

Figure 7. Linear fitting of FLI with domination and γ −domination indices.

There is a very strong (+) correlation between B.P. with DM_1^* and the same can be observed with DM_2, DF^* , DH, DM_1, and DF. Also, there is a very strong (-) correlation with γM_1^*, γM_2, γF^*, γH, γM_1 and γF (Figure 9). There is a very strong (-) correlation between E.C. with DM_1^* and the same can be observed with DM_2, DF^* , DH, DM_1, and DF (Figure 10). While there is a very weak(+) correlation with γM_1^*, γM_2, γH, and a very weak (-) correlation

with γM_1 and γF. E.C. with γF^* closed to independent, the change in E.C. will not affect the change in γF^*. Then domination topological indices have a very strong (+) correlation with ELI, SLI, B.P., and a strong (-) correlation with E.C. While,γ −domination indices have a very strong (-) correlation with B.P and a strong (-) correlation with ELI and SLI except with γM_1, γF it is moderate (-). And γ −domination indices have a very weak (-) correlation with E.C.

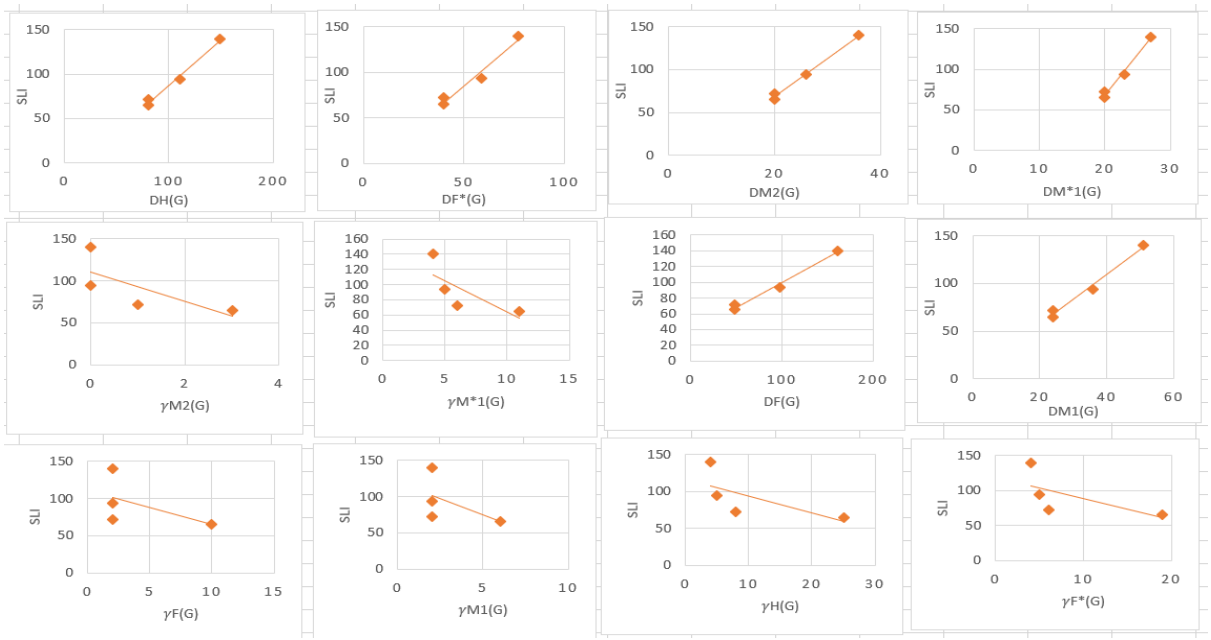

Figure 8. Linear fitting of SLI with domination and γ −domination indices.

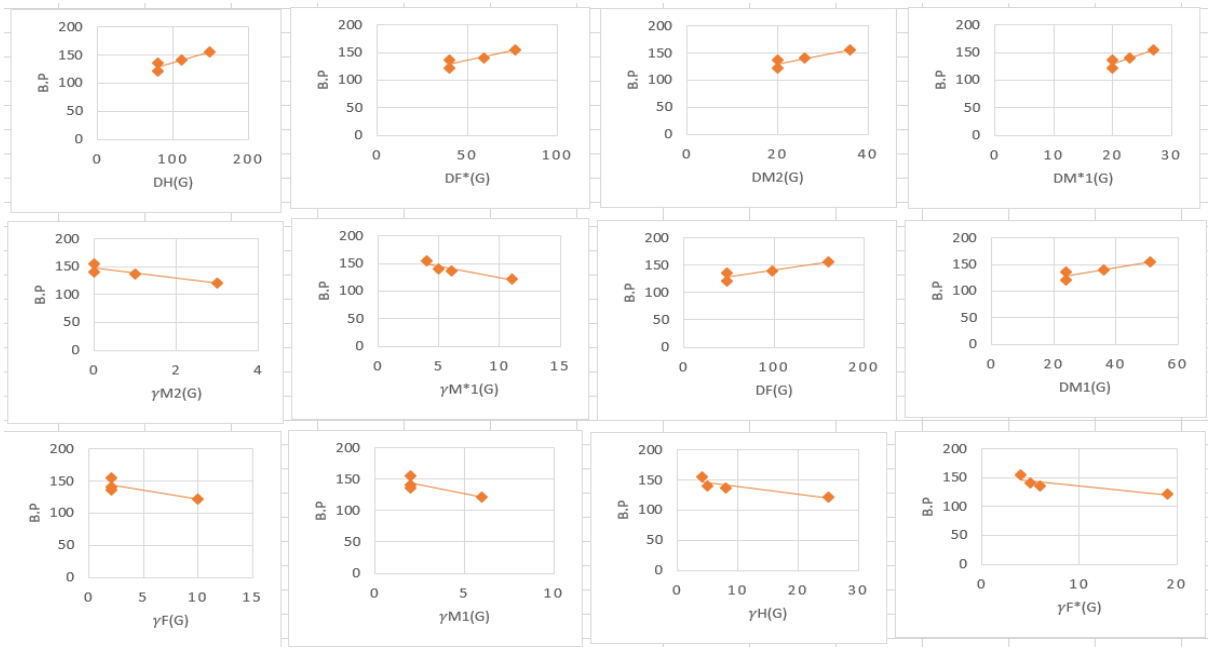

Figure 9. Linear fitting of B.P with domination and γ −domination indices.

4. Conclusions

In this paper, we have studied some of the physicochemical properties of hexane isomers through some indices based on domination degree and domination value. First, we calculate φ_d-polynomial and φ_γ-polynomial with their respective 3D graphs. Then from these polynomials, we compute the domination and γ-domination indices. We found a better

correlation coefficient between domination and γ −domination topological indices and some physicochemical properties of hexane isomers.

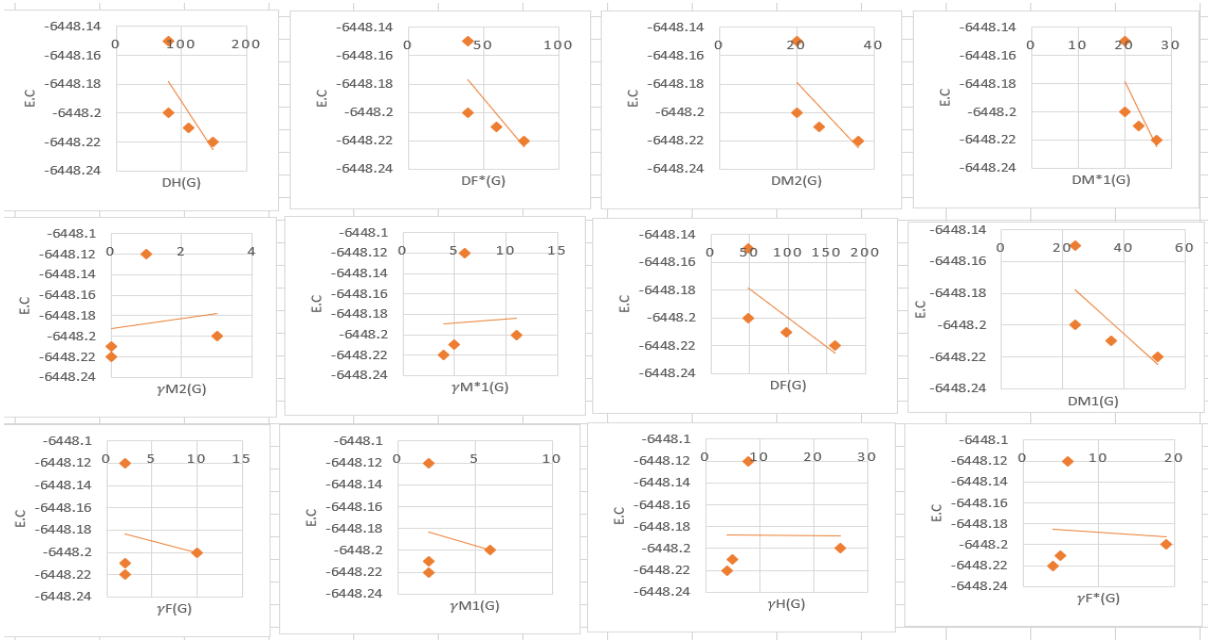

Figure 10. Linear fitting of E.C with domination and γ −domination indices.

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Conflicts of Interest

The authors declare no conflict of interest.

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