Domination Topological Properties of Some Chemical Structures Using φp-Polynomial Approach

Hanan Ahmed, Mohammed Reza Farahani
Department of Mathematics, Yuvaraja's college, University of Mysore, Mysuru, India
Department of Mathematics, Iran University of Science and Technology Narmak, Iran

hananahmed1a@gmail.com; mrfarahani88@gmail.com
Anwar Alwardi, Ruby Salestina M
Department of Mathematics, University of Aden, Yemen
Department of Mathematics, Yuvaraja's college, University of Mysore, Mysuru, India
a_wardi@hotmail.com; ruby.salestina@gmail.com

ABSTRACT

φp-Polynomial is one way to represent a graph algebraically, and it has a major role in theoretical chemistry. It is used in the calculation of the exact values of many topological indices that depend on the P set degree. In this paper, we study the φp-Polynomial by using minimal and minimum dominating sets for Nicotine, Aspirin, and Anthraquinone. Using those φp-Polynomial, some domination and domination topological indices are derived. Also, the results are graphically interpreted.

KEYWORDS: φp-Polynomial, Domination topological indices, Anthraquinone, Nicotine, Aspirin.

INTRODUCTION

Chemical graph theory is one of the branches of mathematical chemistry. Where chemical graph theory is important and necessary for a better understanding and interpretation of the nature of the chemical composition. Recently, the chemical graph theory is used in organizing and arranging the existing problem, because it provides an arrangement of the rules and laws according to specific system and a specific planning. Topological indices can be viewed as molecular descriptors that describe the composition of chemical structures and help predict some of the chemical and physical properties of these structures. Anthraquinone is an aromatic organic compound with the formula C14H8O2. It is a highly crystalline yellow solid that is poorly soluble in water but soluble in hot organic solvents. Hydrogenation gives dihydroanthraquinone (anthrahydroquinone). [13]. Sulfonation with sulfuric acid gives anthraquinone-1-sulfonic acid [16], which reacts with sodium chlorate to give 1-chloro-anthaquinone [17]. Nicotine is a widely used stimulant and a parasympathetic alkaloid, as it is produced naturally from the roots of the nicotine talcum plant, a plant found in the American continent, where it was extracted from the leaves of this plant in 1828 [18, 19, 22]. The pure state of nicotine is an alkaloid that has no color, is volatile, is soluble in water, and is also considered bioactive [22], it can also be absorbed through the skin and mucous membranes in the mouth and nose, as well as in the alveoli [2]. The largest nicotine consumption can be considered through cigarettes, which contain an average of 14 mg per cigarette. It is noted that the amount provided by smoking varies and depends on the quality of the cigarettes and other factors [20]. The cerebral half-life of nicotine is 52 minutes [1, 14, 19, 22]. Aspirin is considered one of the oldest medicines due to its frequent use in various fields of medicine. Aspirin was accepted for back pain in 1903 and 1923 aspirin was used to treat headaches, and it was also used for arthritis in 1933. Studies in 1988 showed that aspirin may be effective in preventing and treating gallstones [10]. Also, there are many studies that have shown beneficial effects on various cancer cases see [3, 4, 11, 15, 21]. Aspirin is considered an anti-headache and insomnia, a pain reliever, and an anti-fever in the case of infectious diseases and against blood clots. A set D⊆V is said to be a dominating set of G, if for any vertex v∈V-D there exists a vertex u∈D such that u and v are adjacent. A dominating-set D={v1;v2;...;vr} is minimal if D vi is not a dominating set [12]. a dominating set of G of minimum cardinality is said a minimum dominating set. A topological index is a numerical parameter of the graph, such that this parameter is the same for the graph which they are isomorphism.

2 BASIC DEFINITIONS

In [6] Hanan Ahmed et al. are introduce the definition of φ_P-polynomial as

Definition 2.1. Let $G=(V;E)$ be a graph, $d_P(v)$ be the P set degree of the vertex v denoted by $d_P(v)=|\{S\subseteq V(G): S \text{ has property } P \text{ and } v\in S\}|$.

The minimum and maximum P set degree of G denote 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 $d_Pm_{i;j}(G)=|\{e=uv: d_P(u)=i;d_P(v)=j\}|$. The φ_P-polynomial define as

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

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

Table 1: Description of some domination and γ-domination topological indices.

Domination (D) and γ-Domination (γD) indices defined on E(G) can be written as

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

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

Table 2: Derivation of domination and domination topological indices from φ_p -Polynomials.

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

In [7, 8, 9] authors have introduced new topological indices called domination and γ-domination topological indices, which are defined as

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

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

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

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 minimum and maximum domination degree of G are denoted by $\delta_d(G)=\delta_d$ and $\Delta_d(G)=\Delta_d$ respectively. In which $\delta_d=min\{d_d(v): v\in V(G)\}$ and $\Delta_d=max\{d_d(v): v\in V(G)\}$.

Definition 2.2. [5] For all vertex v∈V(G) the domination value of v de ne as:

$d\gamma(v)=|\{S\subseteq V(G)$: S is a minimum dominating set and $v\in S\}|$.

We denote the minimum and maximum domination value of a graph G by:

$\delta\gamma(G)=\delta\gamma=\min\{d\gamma(v): v\in V(G)\}$ and $\Delta\gamma(G)=\Delta\gamma=\max\{d\gamma(v): v\in V(G)\}$ respectively.

The γ-domination Zagreb, γ-domination forgotten, γ-domination hyper indices are define as:

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

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

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

3 RESULTS AND DISCUSSION: ANTHRAQUINONE

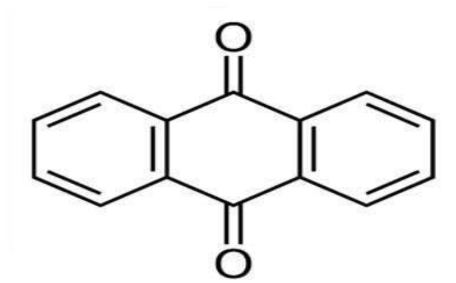

Figure:1 Anthraquinone

Lemma 3.1. The total number of minimal and minimum dominating sets in the molecular graph of anthraquinone is 100 and 57 respectively.

Proof Let G be the molecular graph of anthraquinone. We first divide G into three components C_1, C_2, and C_3. We calculate the minimal dominating sets of each component, so that we get $T_m(C_1)=5$, $T_m(C_2)=7$, and $T_m(C_3)=5$.

Every minimal dominating set of C_1 is added to each minimal dominating set of C_2, and we check for the minimality of the resulting dominating sets. As a result, we get $5\times7=35$ minimal dominating sets, of which 10 are repeated. Hence we get, 25 minimal dominating sets.

Again, every minimal dominating set of C_3 is added to each of the 25 minimal dominating sets, and we check for the minimality of the resulting dominating sets. In this case, we get a total of $5\times25=125$ minimal dominating sets, of which 25 are repeated. In all, there are 100 minimal dominating sets of G. Note that $\gamma(G)=6$, and we have the fact that every minimum dominating set is a minimal dominating set. Out of 100 minimal dominating sets, there are exactly 57 sets whose cardinality is equal to the domination number of G. Hence G has 57 minimum dominating sets.■

To obtain φ_d and φ_γ polynomials of G≈anthraquinone, the table 3 and 4 are very essential.

dd(v)	50	40	30
Number of the vertices	4	9	3

Table 3: Domination degree of the vertices of G

dγ(v)	35	32	25	22	21	16	14
Number of the vertices	1	1	3	2	3	4	2

Table 4: Domination value of the vertices of G.

Theorem 3.2. If G is the molecular graph of anthraquinone, then

$\varphi_d(G;x;y)=x^{30}[y^{30}+4y^{40}+3y^{50}]+x^{40}[7y^{40}+y^{50}]+2x^{50}y^{50}$.

$\varphi_\gamma(G;x;y)=x^{14}[y^{14}+y^{21}+y^{22}+y^{32}+y^{35}]+x^{16}[2y^{16}+4y^{25}+y^{32}+y^{35}]+x^{21}[3y^{22}+y^{35}]+x^{25}+y^{32}$.

Proof. Case 1: Let $d_dm_{ij}(G)=|\{e=uv: d_d(u)=i;d_d(v)=j\}|$.

The edge set of G can be divided into six partitions based on the domination degree of end vertices of each edge as given as follows:

ddmij(G)	(30,30)	(30,40)	(30,50)	(40,40)	(40,50)	(50,50)
Number of the edges	1	4	3	7	1	2

Table 5: Edges partition.

Hence from Table 5, we get

$$\varphi_d(G,x,y)=\sum_{\delta_d\le i\le j\le\Delta_d} d_d m_{ij}(G)x^i y^j = x^{30}[y^{30}+4y^{40}+3y^{50}]+x^{40}[7y^{40}+y^{50}]+2x^{50}y^{50}.$$

<u>Case</u> <u>2:</u> The edge partition depends on the domination value of end vertices of each edge as given in Table 6.

Number of edges	$d_\gamma m_{ij}$
1	*(14,14);(14,21);(14,22); (14,32);(14,35);(16,32); (16,35);(21,35);(25,32)*
2	*(16,16)*

3	*(21,22)*
4	*(16,25)*

Table 6: Edge partition.

So from Table 6, we get

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

$$=x^{14}[y^{14}+y^{21}+y^{22}+y^{32}+y^{35}]+x^{16}[2y^{16}+4y^{25}+y^{32}+y^{35}]+x^{21}[3y^{22}+y^{35}]+x^{25}+y^{32}\blacksquare$$

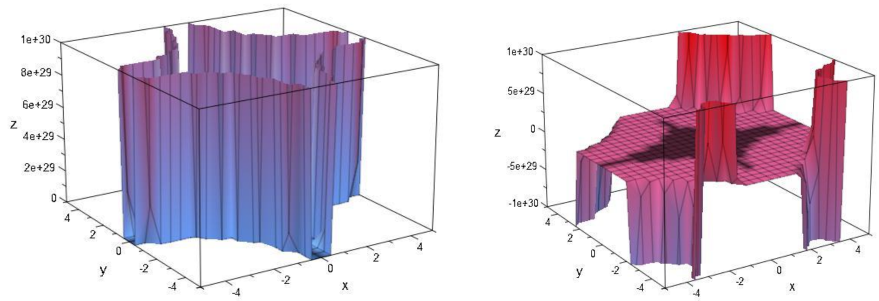

Figure 2. Plotting of (a) φ_d-polynomial and (b) φ_γ-polynomial of Anthraquinone.

Theorem 3.3. Suppose G is the molecular graph of anthraquinone. Then

1. $DM_1^*(G)=1430;\ \gamma M_1(G)=763;$
2. $DF^*(G)=58500;\ \gamma F^*(G)=17749;$
3. $DM_2(G)=28400;\ \gamma M_2(G)=7841;$
4. $DH(G)=115300;\ \gamma H(G)=33431.$

Proof. We have

$\varphi_d(G;x;y)=x^{30}[y^{30}+4y^{40}+3y^{50}]+x^{40}[7y^{40}+y^{50}]+2x^{50}y^{50}.$

Then

$(D_x+D_y)(\varphi_d(G;x;y))=x^{30}[60y^{30}+280y^{40}+240y^{50}]+x^{40}[560y^{40}+90y^{50}]+200x^{50}y^{50};$

$(D_x^2+D_y^2)(\varphi_d(G;x;y))=x^{30}[1800y^{30}+10000y^{40}+10200y^{50}]+x^{40}[22400y^{40}+4100y^{50}]+10000x^{50}y^{50};$

$(D_xD_y)(\varphi_d(G;x;y))=x^{30}[900y^{30}+4800y^{40}+4500y^{50}]+x^{40}[11200y^{40}+2000y^{50}]+5000x^{50}y^{50};$

$(D_x+D_y)^2(\varphi_d(G;x;y))=x^{30}[3600y^{30}+19600y^{40}+19200y^{50}]+x^{40}[44800y^{40}+8100y^{50}]+20000x^{50}y^{50}:$

By using Table 2, we get

$DM_1^*(G)=x^{30}[60y^{30}+280y^{40}+240y^{50}]+x^{40}[560y^{40}+90y^{50}]+200x^{50}y^{50}|_{x=y=1}=1430;$

$DF^*(G)=x^{30}[1800y^{30}+10000y^{40}+10200y^{50}]+x^{40}[22400y^{40}+4100y^{50}]+10000x^{50}y^{50}|_{x=y=1}=58500;$

$DM_2(G)=x^{30}[900y^{30}+4800y^{40}+4500y^{50}]+x^{40}[11200y^{40}+2000y^{50}]+5000x^{50}y^{50}|_{x=y=1}=28400;$

$DH(G)=x^{30}[3600y^{30}+19600y^{40}+19200y^{50}]+x^{40}[44800y^{40}+8100y^{50}]+20000x^{50}y^{50}|_{x=y=1}=115300:$

For γ-domination indices we have,

$\varphi_\gamma(G;x;y)=x^{14}[y^{14}+y^{21}+y^{22}+y^{32}+y^{35}]+x^{16}[2y^{16}+4y^{25}+y^{32}+y^{35}]+x^{21}[3y^{22}+y^{35}]+x^{25}+y^{32}:$

Then

$(D_x+D_y)(\varphi_\gamma(G;x;y))=x^{14}[28y^{14}+35y^{21}+36y^{22}+46y^{32}+49y^{35}]+x^{16}[64y^{16}+164y^{25}+48y^{32}+51y^{35}]$
$+x^{21}[129y^{22}+56y^{35}]+57x^{25}y^{32};$

$(D_x^2+D_y^2)(\varphi_\gamma(G;x;y))=x^{14}[392y^{14}+637y^{21}+680y^{22}+1220y^{32}+1421y^{35}]+x^{16}[1024y^{16}+3524y^{25}+1280y^{32}+1481y^{35}]+x^{21}[2775y^{22}+1666y^{35}]+1649x^{25}y^{32};$

$(D_xD_y)(\varphi_\gamma(G;x;y))=x^{14}[196y^{14}+294y^{21}+308y^{22}+448y^{32}+490y^{35}]+x^{16}[512y^{16}+1600y^{25}$
$+512y^{32}+560y^{35}]+x^{21}[1386y^{22}+735y^{35}]+800x^{25}y^{32};$

$(D_x^2+D_y^2+D_xD_y)(\varphi_\gamma(G;x;y))=x^{14}[784y^{14}+1225y^{21}+1296y^{22}+2116y^{32}+2401y^{35}]$ $+x^{16}[2048y^{16}+6724y^{25}+2304y^{32}+2601y^{35}]+x^{21}[5547y^{22}+3136y^{35}]+3249x^{25}y^{32}$:

By using Table 2, we get

${}_\gamma M_1{}^*(G)=x^{14}[28y^{14}+35y^{21}+36y^{22}+46y^{32}+49y^{35}]+x^{16}[64y^{16}+164y^{25}+48y^{32}+51y^{35}]$ $+x^{21}[129y^{22}+56y^{35}]+57x^{25}y^{32}|_{x=y=1}=763;$

${}_\gamma F^*(G)=x^{14}[392y^{14}+637y^{21}+680y^{22}+1220y^{32}+1421y^{35}]+x^{16}[1024y^{16}+3524y^{25}+1280y^{32}$ $+1481y^{35}]+x^{21}[2775y^{22}+1666y^{35}]+1649x^{25}y^{32}|_{x=y=1}=17749;$

${}_\gamma M_2(G)=x^{14}[196y^{14}+294y^{21}+308y^{22}+448y^{32}+490y^{35}]+x^{16}[512y^{16}+1600y^{25}+512y^{32}+560y^{35}$ $]+x^{21}[1386y^{22}+735y^{35}]+800x^{25}y^{32}|_{x=y=1}=7841;$

${}_\gamma H(G)=x^{14}[784y^{14}+1225y^{21}+1296y^{22}+2116y^{32}+2401y^{35}]+x^{16}[2048y^{16}+6724y^{25}+2304y^{32}$ $+2601y^{35}]+x^{21}[5547y^{22}+3136y^{35}]+3249x^{25}y^{32}|_{x=y=1}=33431.$■

4 RESULTS AND DISCUSSION: NICOTIN

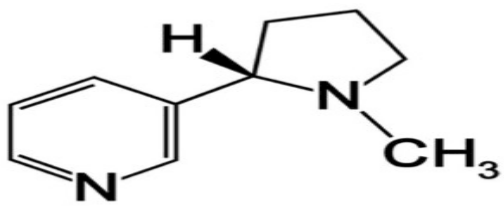

Figure 3: Nicotine

Lemma 4.1. Suppose G is the molecular graph of the nicotine. The total number of a minimal and minimum dominating set is 29 and 6 respectively. To obtain φ_d and φ_γ-polynomials of G, the table 7 and 8 are very essential.

dd(v)	9	10	11	12	14	19
Number of vertices	1	3	2	3	2	1

Table 7: Domination degree of vertices of G.

dγ(v)	0	2	3	6
Number of vertices	3	6	2	1

Table 8: Domination value of vertices of G.

Theorem 4.2. Let G be the molecular graph of nicotine. Then

(i) $\varphi_d(G;x;y)=x^9[2y^{10}+y^{14}]+x^{10}[y^{10}+2y^{12}+y^{14}+y^{19}]+4x^{11}y^{12}+x^{14}y^{14}$;

(ii) $\varphi_\gamma(G;x;y)=y^2+2y^3+3y^6+6x^2y^2+x^3y^3$:

Proof. <u>**Case**</u> <u>**1.**</u> The set of edges that is ended by domination degree can be divided into:

${}_dm_{9;10}=2$, ${}_dm_{9;14}=1$, ${}_dm_{10;10}=1$, ${}_dm_{10;12}=2$, ${}_dm_{10;14}=1$, ${}_dm_{10;19}=1$, ${}_dm_{11;12}=4$, ${}_dm_{14;14}=1$. Now

$$\varphi_d(G,x,y)=\sum_{\delta_d\le i\le j\le\Delta_d} {}_dm_{i,j}(G)x^iy^j={}_dm_{9;10}x^9y^{10}+{}_dm_{9;14}x^9y^{14}+{}_dm_{10;10}x^{10}y^{10}+{}_dm_{10;12}x^{10}y^{12}$$
$$+{}_dm_{10;14}x^{10}y^{14}+{}_dm_{10;19}x^{10}y^{19}+{}_dm_{11;12}x^{11}y^{12}+{}_dm_{14;14}x^{14}y^{14}$$

After putting the value of $d_dm_{i;j}$, we get
$\varphi_d(G;x;y)=x^9[2y^{10}+y^{14}]+x^{10}[y^{10}+2y^{12}+y^{14}+y^{19}]+4x^{11}y^{12}+x^{14}y^{14}$.

<u>Case</u> <u>2:</u> Likewise, the edges whose beginning and end are domination value can be divided as:
$d_\gamma m_{0;2}=1$, $d_\gamma m_{0;3}=2$, $d_\gamma m_{0;6}=3$, $d_\gamma m_{2;2}=6$, $d_\gamma m_{3;3}=1$. As above we get
$\varphi_\gamma(G;x;y)=y^2+2y^3+3y^6+6x^2y^2+x^3y^3$.■

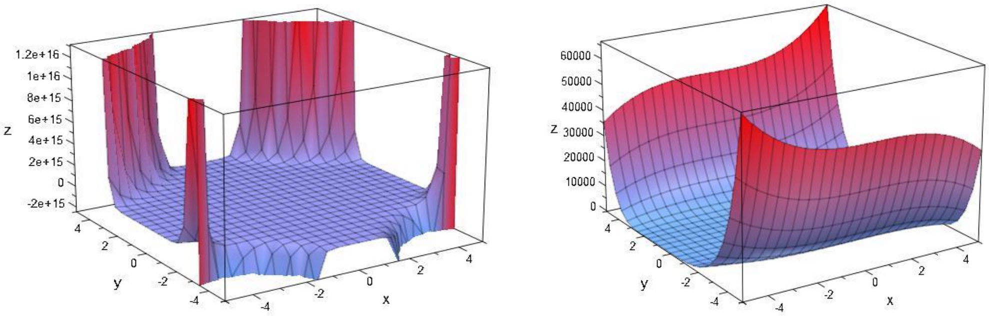

Figure 4. Plotting of (a) φd-polynomial and (b) φγ-polynomial of Nicotine.

Theorem 4.3. Suppose G is the molecular graph of nicotine. Then we have

1. $DM_1^*(G)=298; {}_\gamma M_1(G)=59$,
2. $DF^*(G)=3536; {}_\gamma F^*(G)=196$;
3. $DM_2(G)=1700; {}_\gamma M_2(G)=33$;
4. $DH(G)=6936; {}_\gamma H(G)=262$:

Proof. We have
$\varphi_d(G;x;y)=x^9[2y^{10}+y^{14}]+x^{10}[y^{10}+2y^{12}+y^{14}+y^{19}]+4x^{11}y^{12}+x^{14}y^{14}$;
$\varphi_\gamma(G;x;y)=y^2+2y^3+3y^6+6x^2y^2+x^3y^3$:
Then
$(D_x+D_y)(\varphi_d(G;x;y))=x^9[38y^{10}+23y^{14}]+x^{10}[20y^{10}+44y^{12}+24y^{14}+29y^{19}]+92x^{11}y^{12}+28x^{14}y^{14}$;
$(D_x^2+D_y^2)(\varphi_d(G;x;y))=x^9[362y^{10}+277y^{14}]+x^{10}[200y^{10}+488y^{12}+296y^{14}+461y^{19}]+1060x^{11}y^{12}+392x^{14}y^{14}$;
$(D_xD_y)(\varphi_d(G;x;y))=9x^9[20y^{10}+14y^{14}]+10x^{10}[10y^{10}+24y^{12}+14y^{14}+19y^{19}]+528x^{11}y^{12}+196x^{14}y^{14}$;
$(D_x^2+D_y^2+2D_xD_y)(\varphi_d(G;x;y))=x^9[722y^{10}+529y^{14}]+x^{10}[400y^{10}+968y^{12}+576y^{14}+841y^{19}]+2116x^{11}y^{12}+784x^{14}y^{14}$;
$(D_x+D_y)(\varphi_\gamma(G;x;y))=2y^2+6y^3+18y^6+24x^2y^2+9x^3y^3$;
$(D_x^2+D_y^2)(\varphi_\gamma(G;x;y))+4y^2+18y^3+108y^6+48x^2y^2+18x^3y^3$;$(D_xD_y)(\varphi\ (G;x;y))=24x^2y^2+9x^3y^3$;
$(D_x^2+D_y^2+2D_xD_y)(\varphi_\gamma(G;x;y))=4y^2+18y^3+108y^6+69x^2y^2+36x^3y^3$.
The required result can be obtained using Table 2.■

5. RESULTS AND DISCUSSION: ASPRINI

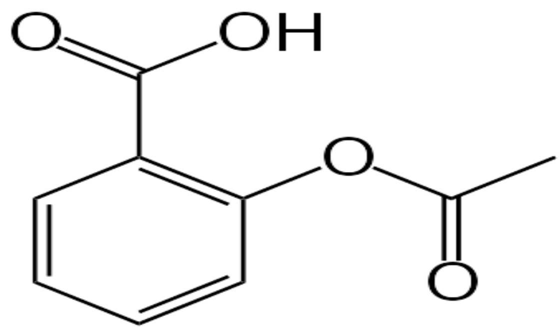

Figure 5: Asprini

Lemma 5.1 Let G be the molecular graph of Aspirin. Then the total number of minimal and minimum dominating sets is 20 and 4 respectively.

To obtain φ_d and φ_γ polynomials of G, molecular graph of Aspirin, the table 9 and 10 are very essential.

$d_d(v)$	6	7	8	10
Number of the vertices	1	1	4	7

Table 9: Domination degree of the vertices of G.

$d_\gamma(v)$	0	1	2	4
Number of the vertices	6	3	2	2

Table 10: Domination value of the vertices of G.

Theorem 5.2. If G is the molecular graph of Aspirin, then
(i) $\varphi_d(G;x;y)=x^6[y^7+y^8+y^{10}]+x^7[y^8+y^{10}]+3x^8y^8+5x^{10}y^{10}$;
(ii) $\varphi_\gamma(G;x;y)=y^9[1+x+x^2]+y^4[5+x]+xy+3xy^2$.

Proof. The edges of the graph can be divided by depending on the domination degree and the domination value of the ends, as in the following table

Number of edges	$d_d m_{i;j}$ *(i;j)*
1	*6;7 & 6;8 & 6;10 & 7;8 & 7;10 & 0;9 & 1;1 & 1;4 & 1;9 & 2;9*
3	*8;8 & 1;2*
5	*10;10 & 0;4*

Table 11: Edges partition.

We get the desired result through definition of φ_P-polynomial and Table 11.■

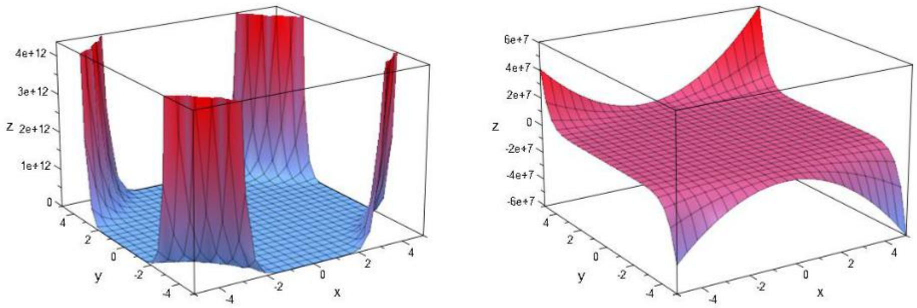

Figure 4. Plotting of (a)φd-polynomial and (b) φγ-Polynomial of Asprini.

Theorem 5.3. Let G be the molecular graph of Aspirin, then

1. $DM_1{}^*(G)=223;{}_{\gamma}M_1{}^*(G)=66,$
2. $DF^*(G)=1967;{}_{\gamma}F^*(G)=359,$
3. $DM_2(G)=968;{}_{\gamma}M_2(G)=38;$
4. $DH(G)=3903;{}_{\gamma}H(G)=438.$

Proof. We have

(i) $\varphi_d(G;x;y)=x^6[y^7+y^8+y^{10}]+x^7[y^8+y^{10}]+3x^8y^8+5x^{10}y^{10};$

(ii) $\varphi_\gamma(G;x;y)=y^9[1+x+x^2]+y^4[5+x]+xy+3xy^2.$

By applying the same method of proof of Theorem 4.3, we get the results.■

6 CONCLUSION

We have studied and computed the properties of some chemical compounds namely anthraquinone, nicotine, and aspirin through domination and gamma domination topological indices. First, we find φ_d polynomial and φ_γ polynomial and their respective 3D graphs. Then we compute the domination and gamma domination indices from these polynomials. It is known that topological indices have the ability to predict some different characteristics, such as the central factor, stability of chemical compounds, boiling point, etc.

REFERENCES

[1] Alkam T, Nabeshima T, Molecular mechanisms for nicotine intoxication, Neuroch Int 2019; 125:117-126.

[2] Baraona LK, Lovelace D, Daniels JL, McDaniel L, Tobacco harms, nicotine pharmacology, and pharmacologic tobacco cessation interventions for women, J Midwifery Womens Health 2017;62:253-269.

[3] Bardia A et al. Effect of aspirin and other NSAIDs on postmenopausal breast cancer incidence by hormone receptor status: Results from a prospective cohort study, Breast Cancer Res Treat. 2011;126(1):149-55.

[4] Dhillon PK, et al. Longterm aspirin use and the risk of total, high-grade, regionally advanced and lethal prostate cancer in a prospective cohort of health professionals, 1988-2006, Int J Cancer 2011;128(10): 2444-52.

[5] Eunjeong Y., Domination value in graph, arXiv:1109.6277v2 [math.CO] 1 Mar 2012.

[6] Hanan Ahmed., A. Alwardi, R. Salestina M, Domination, Domination Topological Indices and φ_p-Polynomial of Some Chemical Structures Applied for the Treatment of COVID-19 Patients,

Biointerface research in applied chemistry, 5, 2021, 13290 – 13302 DOI: 10.33263/BRIAC115.1329013302
[7] Hanan Ahmed. A. Alwardi, R. Salestina M., On Domination Zagreb Indices of Graphs, International Journal of Analysis and Applications 19(1) 47-64 (2020).
[8] Hanan Ahmed., A. Alwardi, R. Salestina M., N.D. Soner, Forgotten Domination and Hyper Domination Indices of Graphs, Journal of discrete mathematical sciences and cryptorgraphy, In Press DOI:10.1080/09720529.2021.1885805
[10] Hanan Ahmed., A. Alwardi, R. Salestina M., Domination Topological Indices and Their Polynomials of a Fire y Graph, Journal of discrete mathematical sciences and cryptorgraphy, In Press DOI:10.1080/09720529.2021.1882155
[11] Heller FR, Sludge, gallstones and aspirin, Acta Gastroenterol Belg. 1990;53(1):16-21.
[12] Mascitelli L, Pezzetta F, Sullivan JL, Aspirin-associated iron loss as an anticancer mechanism, Med Hypotheses 2010;74(1): 78-80.
[13] Jean-Franois Couturier, Romain Letourneur, Mathieu Liedlo, On the number of minimal dominating sets on some graph classes, Theoretica Computer Science.562, (2015), 634642.
[14] Macleod, L. C. Allen, C. F. H.Benzanthrone, Organic Syntheses,(1934) 14: 4 doi:10.15227/orgsyn.014.0004
[15] Marsot A, Simon N, Nicotine and cotinine levels with electronic cigarette: a review, Int J Toxicol 2016;35:179-185.
[16] Rothwell PM, Fowkes FG, Belch JF, Ogawa H, Warlow CP, Meade TW, Effect of daily aspirin on long-term risk of death due to cancer: Analysis of individual patient data from randomised trials, Lancet 2011;377(9759): 31-41.
[17] Scott, W. J. Allen, C. F. H. Potassium Anthraquinone--Sulfonate, Organic Syntheses,(1938), 18, 72 doi:10.15227/orgsyn.018.0072
[18] Scott, W. J.; Allen, C.F. H.-Chloroanthraquinone, (1938), 18: 15. doi:10.15227/orgsyn.018.0015
[19] Sieber M, Neuroprotective properties of nicotine, Curr Med Chem 2012;19:292-297.
[20] Siqueira LM, Nicotine and tobacco as substances of abuse in children and adolescents, Pediatrics. 2017;139:1-15.
[21] Valentine G, Sofuoglu M, Cognitive effects of nicotine: recent progress, Cur Neuropharmacol 2018;16:403-414.
[22] Van Dyke AL, M.L. Cote, G. Prysak, G.B. Claeys, A.S. Wenzlaff, A.G. Schwartz. Regular adult aspirin use decreases the risk of non-small cell lung cancer among women, Cancer Epidemiol Biomarkers Prev 2008;17(1):148-57.
[23] Zarrindasta M, Khakpai F, The modulatory role of nicotine on cognitive and non-cognitive functions, Brain Research 2019;1710:92-101.