




**FULL PAPER**

# Domination topological properties of some chemical structures using $\varphi_p$ -Polynomial approach

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$\varphi_p$ -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  $\varphi_p$ -Polynomial by using minimal and minimum dominating sets for Nicotine, Aspirin, and Anthraquinone. Using those  $\varphi_p$ -Polynomials, some domination and domination topological indices are derived. Also, the results are graphically interpreted.

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**KEYWORDS** $\varphi_p$ -Polynomial; domination topological indices; anthraquinone; nicotine; aspirin.**Introduction**

Chemical graph theory is one of the branches of mathematical chemistry, where it 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 a specific systems and 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  $C_{14}H_8O_2$ . 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, 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, 24-35]. 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 in 1923 aspirin was

used to treat headaches, and it was also used for arthritis in 1933. Studies in 1988 showed that aspirin could 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 is against blood clots. A set  $D \subseteq V$  is said to be a dominating set of  $G$ , 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  $D = \{v_1, v_2, \dots, v_r\}$  is minimal if  $D - v_i$  is not a dominating set [12]. A dominating set of  $G$  of minimum cardinality is said to be 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 is isomorphism.

### Basic definitions

**TABLE 1** Description of some domination and  $\gamma$ -domination topological indices

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

**TABLE 2** Derivation of domination and domination topological indices from  $\phi_P$ -Polynomials

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

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

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

In [7-9] authors have introduced new topological indices called domination and  $\gamma$ -

In Hanan Ahmed *et al.* [6] the definition of  $\phi_P$ -polynomial is introduced 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  $\phi_P$ -polynomial is defined as

$$\phi_P(G, x, y) = \sum_{\delta_P \leq i \leq j \leq \Delta_P} d_{Pm_{i,j}}(G) x^i y^j.$$

Domination (D) and  $\gamma$ -Domination ( $\gamma$ D) indices defined on  $E(G)$ , which can be written as TABLE 1 follows:

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

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

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  $v \in V(G)$ , the domination value of  $v$  define as:  $d_\gamma(v) = |\{S \subseteq V(G) : S \text{ is a minimum dominating set and } v \in S\}|$ .

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  $\gamma$ -domination Zagreb,  $\gamma$ -domination forgotten,  $\gamma$ -domination hyper indices are defined as:

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

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

$$\gamma F(G) = \sum_{v \in V(G)} d_\gamma^3(v),$$

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

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

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

## Results and discussion: Anthraquinone

**TABLE 3** Domination degree of the vertices of  $G$ . (\*)

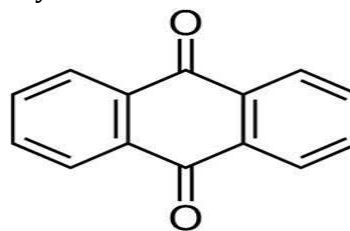
$d_d(v)$	50	40	30
Number of the vertices	4	9	3

(\*) To obtain  $\phi_d$  and  $\phi_\gamma$  polynomials of  $G \approx$  anthraquinone, Tables 3 and 4 are very essential

**TABLE 4** Domination value of the vertices of  $G$

$d_\gamma(v)$	35	32	25	22	21	16	14
Number of the vertices	1	1	3	2	3	4	2

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



**FIGURE1** Anthraquinone

**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  $5 \times 7 = 35$  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  $5 \times 25 = 125$  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. ■

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

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

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

**TABLE 5** Edges partition

$d_{am_{ij}}(G)$	(30,30)	(30,40)	(30,50)	(40,40)	(40,50)	(50,50)
Number of the edges	1	4	3	7	1	2

Hence from Table 5, we get

$$\varphi_d(G, x, y) = \sum_{\delta_i \leq i \leq j \leq \Delta_d} d_{am_{ij}}(G) x^i y^j$$

$$= x^{30}[y^{30} + 4y^{40} + 3y^{50}] + x^{40}[7y^{40} + y^{50}] + 2x^{50}y^{50}.$$

**TABLE 6** Edge partition

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)

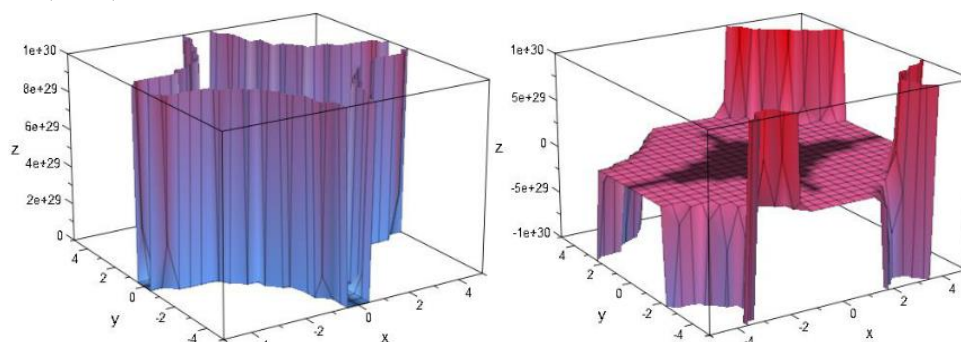
So, from Table 6, we get

$$\varphi_\gamma(G, x, y) = \sum_{\delta_\gamma \leq i \leq j \leq \Delta_\gamma} d_{\gamma m_{ij}}(G) x^i y^j = x^{14}[y^{14} + y^{21} + y^{22} + y^{32} + y^{35}] + x^{16}[2y^{16} + 4y^{25} + y^{32} + y^{35}] + x^{21}[3y^{22} + y^{35}] + x^{25} + y^{32}.$$

**Proof. Case 1:** Let  $d_{am_{ij}}(G) = |\{e = uv : d_a(u) = i, d_a(v) = j\}|$ .

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 Table 5 follows:

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



**FIGURE 2** Plotting of (a)  $\varphi_d$ -polynomial and (b)  $\varphi_\gamma$ -polynomial of Anthraquinone

**Theorem 3.3.** Suppose  $G$  is the molecular graph of anthraquinone, then

- $DM_1^*(G) = 1430, \gamma M_1(G) = 763,$
- $DF^*(G) = 58500, \gamma F^*(G) = 17749,$
- $DM_2(G) = 28400, \gamma M_2(G) = 7841,$
- $DH(G) = 115300, \gamma H(G) = 33431.$

**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

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

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

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

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

$$+ x^{40}[44800y^{40} + 8100y^{50}] + 20000x^{50}y^{50}$$

By using Table 2, we get

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

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

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  $\gamma$ -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

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

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

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

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

By using Table 2, we get

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

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

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

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

= 33431.

### Results and discussion: Nicotin

**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  $\varphi_d$  and  $\varphi_\gamma$ -polynomials of G, Tables 7 and 8 are very essential.

**TABLE 7** Domination degree of vertices of G.

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

**TABLE 8** Domination value of vertices of G

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



**FIGURE 3** Nicotin

**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. Case 1.** The set of edges that is ended by domination degree can be divided into:

$$d_{am_{9,10}}=2, \quad d_{am_{9,14}}=1, \quad d_{am_{10,10}}=1, \quad d_{am_{10,12}}=2, \\ d_{am_{10,14}}=1, \quad d_{am_{10,19}}=1, \quad d_{am_{11,12}}=4, \quad d_{am_{14,14}}=1.$$

Now

$$\varphi_d(G, x, y) = \sum_{\delta_j \leq i \leq j \leq \Delta_d} d_{am_{i,j}}(G)x^i y^j \\ = d_{am_{9,10}}x^9y^{10} + d_{am_{9,14}}x^9y^{14} + d_{am_{10,10}}x^{10}y^{10} + \\ d_{am_{10,12}}x^{10}y^{12} + d_{am_{10,14}}x^{10}y^{14} + d_{am_{10,19}}x^{10}y^{19} \\ + d_{am_{11,12}}x^{11}y^{12} + d_{am_{14,14}}x^{14}y^{14}$$

After putting the value of  $d_{am_{i,j}}$  we get

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

**Case 2:** 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

$$\varphi_{\gamma}(G,x,y)=y^2+2y^3+3y^6+6x^2y^2+x^3y^3. \blacksquare$$

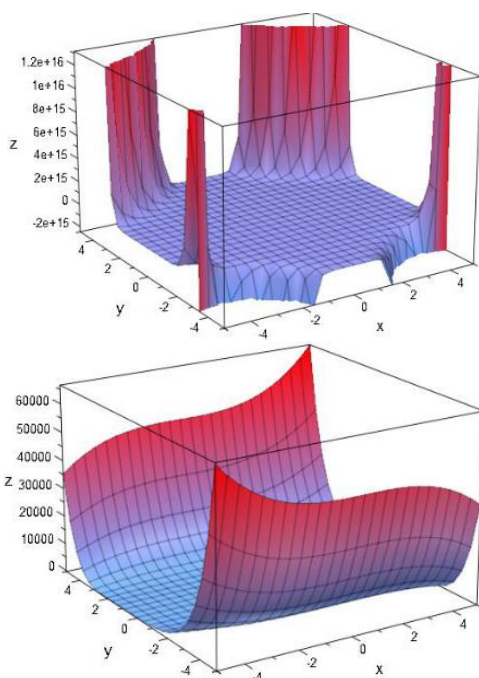
**Theorem 4.3.** Suppose  $G$  is the molecular graph of nicotine. Then, we have

$$1. DM_1^*(G)=298, M_1(G)=59,$$

$$2. DF^*(G)=3536, \gamma F^*(G)=196,$$

$$3. DM_2(G)=1700, \gamma M_2(G)=33,$$

$$4. DH(G)=6936, \gamma H(G)=262:$$



**FIGURE 4** Plotting of (a)  $\varphi_d$ -polynomial and (b)  $\varphi_{\gamma}$ -polynomial of Nicotine

**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

$$(D_x+D_y)(\varphi_d(G,x,y))=x^9[38y^{10}+23y^{14}]+x^{10}[20y^{10}$$

$$+44y^{12}+24y^{14}+29y^{19}]+92x^{11}y^{12}+28x^{14}y^{14},$$

$$(D_x^2+D_y^2)(\varphi_d(G,x,y))=x^9[362y^{10}+277y^{14}]$$

$$+x^{10}[200y^{10}+488y^{12}+296y^{14}+461y^{19}]$$

$$+1060x^{11}y^{12}+392x^{14}y^{14},$$

$$(D_xD_y)(\varphi_d(G,x,y))=9x^9[20y^{10}+14y^{14}]$$

$$+10x^{10}[10y^{10}+24y^{12}+14y^{14}+19y^{19}]$$

$$+528x^{11}y^{12}+196x^{14}y^{14},$$

$$(D_x^2+D_y^2+2D_xD_y)(\varphi_d(G,x,y))=x^9[722y^{10}+529y^{14}]$$

$$+x^{10}[400y^{10}+968y^{12}+576y^{14}+841y^{19}]$$

$$+2116x^{11}y^{12}+784x^{14}y^{14},$$

$$(D_x+D_y)(\varphi_{\gamma}(G,x,y))=2y^2+6y^3+18y^6+24x^2y^2+9x^3y^3,$$

$$(D_x^2+D_y^2)(\varphi_{\gamma}(G,x,y))+4y^2+18y^3+108y^6$$

$$+48x^2y^2+18x^3y^3,$$

$$(D_xD_y)(\varphi_{\gamma}(G,x,y))=24x^2y^2+9x^3y^3,$$

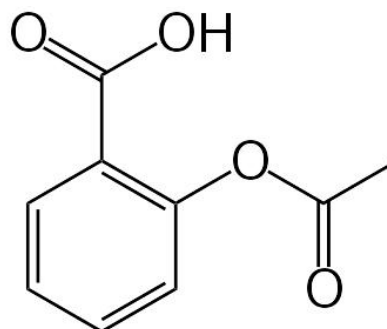
$$(D_x^2+D_y^2+2D_xD_y)(\varphi_{\gamma}(G,x,y))=4y^2+18y^3$$

$$+108y^6+69x^2y^2+36x^3y^3.$$

The required result can be obtained using Table 2. ■

## Results and discussion: Aspirin

**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.



**FIGURE 5** Aspirin

To obtain  $\varphi_d$  and  $\varphi_{\gamma}$  polynomials of  $G$ , molecular graph of Aspirin, Tables 9 and 10 are very essential.

**TABLE 9** Domination degree of the vertices of  $G$

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

**TABLE 10** Domination value of the vertices of  $G$

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

**Theorem 5.2.** If  $G$  is the molecular graph of Aspirin, then

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

$$+5x^{10}y^{10},$$

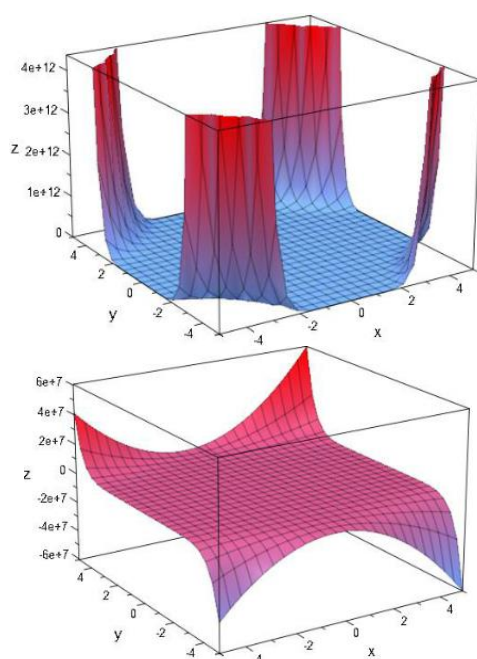
$$(ii) \varphi_{\gamma}(G,x,y)=y^9[1+x+x^2]+y^4[5+x]+xy+3xy^2.$$

**Proof.** The edges of the graph can be divided by depending on the domination degree and

**TABLE 11** Edges partition

Number of edges	$d_{am_{ij}}(i,j)$
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

We get the desired result through definition of  $\varphi_P$ -polynomial and Table 11.■



**FIGURE 6** Plotting of (a) $\varphi_d$ -polynomial and (b)  $\varphi_{\gamma}$ -Polynomial of Aspirin

**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.■

the domination value of the ends, as represented in the Table 11 below.

## 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 found  $\varphi_d$  polynomial and  $\varphi_{\gamma}$  polynomial and their respective 3D graphs (Figures 2, 4 and 6). Then we computed 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.

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