

FULL PAPER

Domination topological properties of carbidopa-levodopa used for treatment Parkinson's disease by using φP -polynomial

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In medical science, pharmacology, chemical, pharmaceutical properties of molecular structure are essential for drug preparation and design. These properties can be studied by using domination topological indices calculation. In this research work, we establish the topological properties of levodopa-carbidopa drug given to people with Parkinson's disease by using the domination of topological indices and domination indices. We determine the φP -polynomial for the chemical structures of levodopa and carbidopa. Also, the results are graphically interpreted.

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Introduction

Chemical graph theory is one of the branches of mathematical chemistry. The importance of chemical graph theory lies in understanding and explaining the nature of the chemical composition, as it was used in organizing the current problem because it determines the arrangement of rules and laws according to a specific system and planning. The atoms are represented as the vertices and the chemical bonds between the atoms are the edges connecting these vertices. Topological indicators are molecular descriptors that describe the composition of chemical structures and help predict some of the chemical and physical properties of these structures. A set D sub set of V is said to be a dominating set of a graph G , if for any vertex $v \in V - D$ there exists a vertex $u \in D$ such that u and v are adjacent. For more details on domination in graphs, see [5,6,7,11,18-28]. A dominating set $D = \{v_1, v_2, \dots, v_r\}$ is minimal if $D - v_i$ is not a dominating set [10]. A dominating set of G of minimum cardinality is said to be a minimum dominating set.

Definition 1.1. [12] For each vertex $v \in V(G)$, the domination degree is denoted by $d_d(v)$ and defined as the number of minimal dominating sets of G which contains v .

Hanan Ahmed et al. [12] have introduced new topological indices called domination Zagreb indices which are based on the minimal dominating sets defined as:

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

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

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

Where $d_d(v)$ is the domination degree of the vertex v . The total number of minimal dominating sets of G is denoted as $T_m(G)$ [12]. The forgotten domination, hyper domination and modified forgotten domination indices of graphs [13] are defined as:

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

Definition 1.2. [14]

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

Researchers have introduced new topological indices called γ -domination topological indices [14], which are defined as:

$$\begin{aligned}\gamma M_1(G) &= \sum_{v \in V(G)} d_\gamma^2(v), \\ \gamma M_2(G) &= \sum_{uv \in E(G)} d_\gamma(u)d_\gamma(v), \\ \gamma F(G) &= \sum_{v \in V(G)} d_\gamma^3(v),\end{aligned}$$

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

Hanan Ahmed et al., introduce the Definition of φ_P -polynomial as follows:

Definition 1.3. Let $G = (V, E)$ be a graph, $d_P(v)$ be the P set degree of the vertex v denoted by [14]:

$d_P(v) = |\{S \subseteq V(G) : S \text{ has property } P \text{ and } v \in S\}|$. The minimum and maximum P set degree of G are 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

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

TABLE 1 Description of some domination and domination topological indices

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

TABLE 2 Derivation of domination and domination topological indices from φ_P -polynomials

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

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

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

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

Here,

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

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

For more information on topological indices and polynomial of graph see [1,2,3,4,9,8,15,16,17].

Results and discussion

Levodopa was developed over 30 years ago and is often considered the appropriate standard for Parkinson's treatment. Levodopa works by crossing the blood-brain barrier, where it is converted to dopamine. The blood enzymes break down most of the levodopa before it reaches the brain. For this reason, levodopa is combined with an enzyme inhibitor called carbidopa. The addition of carbidopa prevents levodopa from being metabolized in the gastrointestinal tract and liver.

In this paper, we used the notations G=molecular graph of levodopa and H=molecular graph of carbidopa.

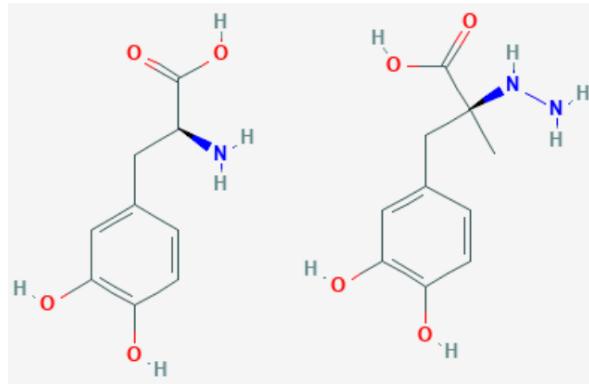


FIGURE 1 Chemical structure of (a) Levodopa C₉H₁₁N O₄ (b) Carbidopa C₁₀H₁₄N₂O₄

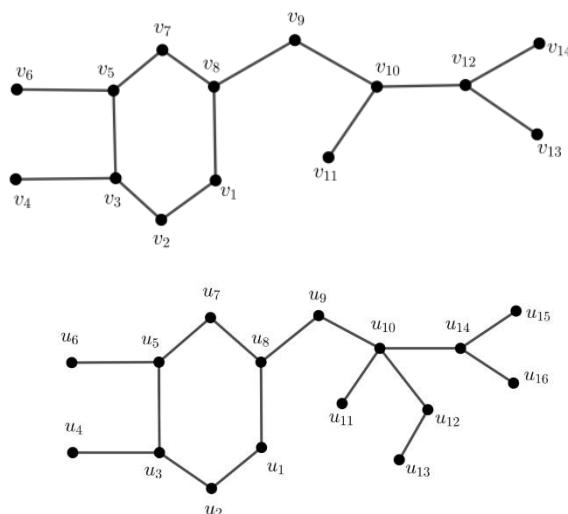


FIGURE 2 Molecular graph of (a) Levodopa C₉H₁₁N O₄ (b) Carbidopa C₁₀H₁₄N₂O₄

Lemma 2.1. Let G and H be the molecular graphs of levodopa and carbidopa, respectively. Then, T_m(G)=49, T_m(H)=96 and there are 6 and 10 minimum dominating sets in the molecular graphs of levodopa and carbidopa, respectively

Proof. Let G be the molecular graph of levodopa C₉H₁₁N O₄. The minimal dominating sets of G are:

$$D_1=\{v_1, v_3, v_5, v_{10}, v_{12}\}, D_2=\{v_1, v_4, v_5, v_{10}, v_{12}\},$$

$$D_3=\{v_1, v_3, v_6, v_7, v_{10}, v_{12}\},$$

$$D_4=\{v_1, v_4, v_6, v_7, v_{10}, v_{12}\}, D_5=\{v_3, v_5, v_8, v_{10}, v_{12}\},$$

$$D_6=\{v_3, v_6, v_8, v_{10}, v_{12}\},$$

$$D_7=\{v_2, v_4, v_5, v_8, v_{10}, v_{12}\},$$

$$D_8=\{v_2, v_4, v_6, v_8, v_{10}, v_{12}\},$$

$$D_9=\{v_2, v_3, v_5, v_7, v_{10}, v_{12}\},$$

$$D_{10}=\{v_2, v_3, v_6, v_7, v_{10}, v_{12}\},$$

$$D_{11}=\{v_2, v_4, v_5, v_7, v_{10}, v_{12}\},$$

$$D_{12}=\{v_2, v_4, v_6, v_7, v_{10}, v_{12}\},$$

$$D_{13}=\{v_1, v_3, v_5, v_{10}, v_{13}, v_{14}\},$$

$$D_{14}=\{v_1, v_4, v_5, v_{10}, v_{13}, v_{14}\},$$

$$D_{15}=\{v_1, v_3, v_6, v_7, v_{10}, v_{13}, v_{14}\},$$

$$D_{16}=\{v_1, v_4, v_6, v_7, v_{10}, v_{13}, v_{14}\},$$

$$D_{17}=\{v_3, v_5, v_8, v_{10}, v_{13}, v_{14}\},$$

$$D_{18}=\{v_3, v_6, v_8, v_{10}, v_{13}, v_{14}\},$$

$$\begin{aligned} D_{19} &= \{v_2, v_4, v_5, v_8, v_{10}, v_{13}, v_{14}\}, \\ D_{20} &= \{v_2, v_4, v_6, v_8, v_{10}, v_{13}, v_{14}\}, \\ D_{21} &= \{v_2, v_3, v_5, v_7, v_{10}, v_{13}, v_{14}\}, \end{aligned}$$

$$\begin{aligned} D_{22} &= \{v_2, v_3, v_6, v_7, v_{10}, v_{13}, v_{14}\}, \\ D_{23} &= \{v_2, v_4, v_5, v_7, v_{10}, v_{13}, v_{14}\}, \\ D_{24} &= \{v_2, v_4, v_6, v_7, v_{10}, v_{13}, v_{14}\}, \end{aligned}$$

$$D_{25} = \{v_1, v_3, v_5, v_9, v_{11}, v_{12}\},$$

$$D_{26} = \{v_1, v_4, v_5, v_9, v_{11}, v_{12}\},$$

$$D_{27} = \{v_1, v_3, v_6, v_7, v_9, v_{11}, v_{12}\},$$

$$D_{28} = \{v_1, v_4, v_6, v_7, v_9, v_{11}, v_{12}\},$$

$$D_{29} = \{v_3, v_5, v_8, v_{11}, v_{12}\},$$

$$D_{30} = \{v_3, v_6, v_8, v_{11}, v_{12}\},$$

$$D_{31} = \{v_2, v_4, v_5, v_9, v_{11}, v_{12}\},$$

$$D_{32} = \{v_2, v_4, v_6, v_8, v_9, v_{11}, v_{12}\},$$

$$D_{33} = \{v_2, v_3, v_5, v_9, v_{11}, v_{12}\},$$

$$D_{34} = \{v_2, v_3, v_6, v_7, v_9, v_{11}, v_{12}\},$$

$$D_{35} = \{v_2, v_4, v_6, v_7, v_9, v_{11}, v_{12}\},$$

$$D_{36} = \{v_1, v_3, v_5, v_9, v_{11}, v_{13}, v_{14}\},$$

$$D_{37} = \{v_1, v_4, v_5, v_9, v_{11}, v_{13}, v_{14}\},$$

$$D_{38} = \{v_1, v_3, v_6, v_7, v_9, v_{11}, v_{13}, v_{14}\},$$

$$D_{39} = \{v_1, v_4, v_6, v_7, v_9, v_{11}, v_{13}, v_{14}\},$$

$$D_{40} = \{v_3, v_5, v_8, v_{11}, v_{13}, v_{14}\},$$

$$D_{41} = \{v_3, v_6, v_8, v_{11}, v_{13}, v_{14}\},$$

$$D_{42} = \{v_2, v_4, v_5, v_9, v_{11}, v_{13}, v_{14}\},$$

$$D_{43} = \{v_2, v_4, v_6, v_8, v_{11}, v_{13}, v_{14}\},$$

$$D_{44} = \{v_2, v_3, v_5, v_9, v_{11}, v_{13}, v_{14}\},$$

$$D_{45} = \{v_2, v_3, v_6, v_7, v_9, v_{11}, v_{13}, v_{14}\},$$

$$D_{46} = \{v_2, v_4, v_5, v_9, v_{11}, v_{13}, v_{14}\},$$

$$D_{47} = \{v_2, v_4, v_6, v_7, v_9, v_{11}, v_{13}, v_{14}\},$$

$$D_{48} = \{v_2, v_4, v_5, v_8, v_{11}, v_{12}\},$$

$$D_{49} = \{v_2, v_4, v_5, v_8, v_{11}, v_{13}, v_{14}\},$$

Note that among 49 minimal dominating sets, there are 6 minimum dominating sets. Similarly, if H be the molecular graph of carbidopa $C_{10}H_{14}N_2O_4$, one can get 96, 10 minimal and minimum dominating sets, respectively.

From Lemma 2.1, Definition 1.1 and Definition 1.2, we get, if $v_i \in V(G)$ then:

$$\begin{aligned} d_d(v_1) &= 16, d_d(v_2) = 24, d_d(v_3) = 24, d_d(v_4) = 24, \\ d_d(v_5) &= 24, d_d(v_6) = 24, d_d(v_7) = 20, d_d(v_8) = 16, \\ d_d(v_9) &= 17, d_d(v_{10}) = 24, d_d(v_{11}) = 24, d_d(v_{12}) = 24, \\ d_d(v_{13}) &= 24, d_d(v_{14}) = 24, d\gamma(v_1) = 2, d\gamma(v_2) = 0, \end{aligned}$$

$$\begin{aligned} d\gamma(v_3) &= 5, d\gamma(v_4) = 1, d\gamma(v_5) = 4, d\gamma(v_6) = 1, \\ d\gamma(v_7) &= 0, d\gamma(v_8) = 4, d\gamma(v_9) = 0, d\gamma(v_{10}) = 4, \\ d\gamma(v_{11}) &= 2, d\gamma(v_{12}) = 6, d\gamma(v_{13}) = 0, d\gamma(v_{14}) = 0 \end{aligned}$$

Similarly, if $u \in V(H)$ we get

$$\begin{aligned} d_d(u_1) &= 32, d_d(u_2) = 48, d_d(u_3) = 48, d_d(u_4) = 48, \\ d_d(u_5) &= 48, d_d(u_6) = 48, d_d(u_7) = 40, d_d(u_8) = 32, \\ d_d(u_9) &= 32, d_d(u_{10}) = 48, d_d(u_{11}) = 48, d_d(u_{12}) = 48, \\ d_d(u_{13}) &= 48, d_d(u_{14}) = 48, d_d(u_{15}) = 48, d_d(u_{16}) = 48, \\ d\gamma(u_1) &= 4, d\gamma(u_2) = 0, d\gamma(u_3) = 8, d\gamma(u_4) = 2, \\ d\gamma(u_5) &= 7, d\gamma(u_6) = 3, d\gamma(u_7) = 0, d\gamma(u_8) = 6, \\ d\gamma(u_9) &= 0, d\gamma(u_{10}) = 8, d\gamma(u_{11}) = 2, d\gamma(u_{12}) = 4, \\ d\gamma(u_{13}) &= 6, d\gamma(u_{14}) = 10, d\gamma(u_{15}) = 0, d\gamma(u_{16}) = 0. \end{aligned}$$

Theorem 2.2. If G is the molecular graph of levodopa, then

$$\varphi_d(G, x, y) = [8x^{24} + x^{20} + x^{16} + x^{17}]y^{24} + [y^{16} + y^{17} + y^{20}]x^{16},$$

$$\varphi_\gamma(G, x, y) = 2y^6 + y^5 + 4y^4 + y^2 + [y^4 + y^5]x + 2x^2y^4 + [y^5 + y^6]x^4$$

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

The edge set of G can be divided into seven partitions based on the domination degree of end vertices of each edge as given as in Table 3, then

$$\varphi_d(G, x, y) = [8x^{24} + x^{20} + x^{16} + x^{17}]y^{24} + [y^{16} + y^{17} + y^{20}]x^{16},$$

Case 2: Let $d_\gamma m_{ij}(G) = |\{e = uv : d_\gamma(u) = i, d_\gamma(v) = j\}|$. The edge partition depends on the domination value of end vertices of each edge as given as in Table 4, then

$$\varphi_\gamma(G, x, y) = 2y^6 + y^5 + 4y^4 + y^2 + [y^4 + y^5]x + 2x^2y^4 + [y^5 + y^6]x^4 \blacksquare$$

Theorem 2.3. Suppose G is the molecular graph of levodopa. Then

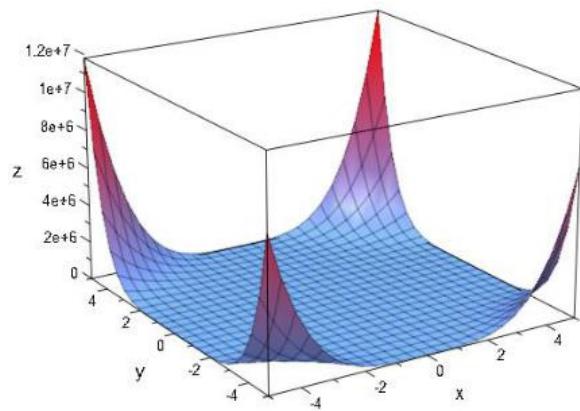
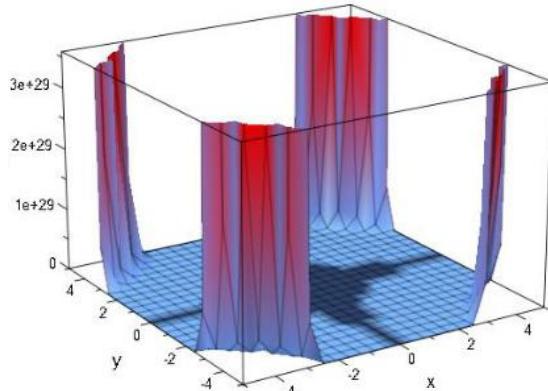
1. $DM_1^*(G) = 610, \gamma M_1^*(G) = 77,$
2. $DF^*(G) = 13602, \gamma F^*(G) = 341,$
3. $DM_2(G) = 6728, \gamma M_2(G) = 69,$
4. $DH(G) = 27058, \gamma H(G) = 479,$
5. $DM_1(G) = 6961, \gamma M_1(G) = 119,$
6. $DF(G) = 159345, \gamma F(G) = 542.$

TABLE 3 Edges partition

d_{ij}	(24, 24)	(20, 24)	(16, 24)	(17, 24)	(16, 16)	(16, 17)	(16, 20)
Number of edges	8	1	1	1	1	1	1

TABLE 4 Edges partition

d_{ij}	(0, 6)	(0, 5)	(0, 4)	(0, 2)	(1, 4)	(1, 5)	(2, 4)	(4, 5)	(4, 6)
Number of edges	2	1	4	1	1	1	2	1	1

**FIGURE 3** Plotting of (a) φ_d -polynomial and (b) φ_γ -polynomial of molecular graph of levodopa

Proof. We have $\varphi_d(G, x, y) = [8x^{24} + x^{20} + x^{16} + x^{17}]y^{24} + [y^{16} + y^{17} + y^{20}]x^{16}$

Then

$$(D_x + D_y)(\varphi_d(G, x, y)) = [384x^{24} + 44x^{20} + 40x^{16} + 41x^{17}]y^{24} + [32y^{16} + 33y^{17} + 36y^{20}]x^{16},$$

$$(D_x^2 + D_y^2)(\varphi_d(G, x, y)) = [9216x^{24} + 976x^{20} + 832x^{16} + 865x^{17}]y^{24} + [512y^{16} + 545y^{17} + 656y^{20}]x^{16},$$

$$(D_x D_y)(\varphi_d(G, x, y)) = [4608x^{24} + 480x^{20} + 384x^{16} + 40x^{17}]y^{24} + [256y^{16} + 272y^{17} + 320y^{20}]x^{16},$$

$$(D_x + D_y)^2(\varphi_d(G, x, y)) = [18432x^{24} + 1936x^{20} + 1600x^{16} + 1681x^{17}]y^{24} + [1024y^{16} + 1089y^{17} + 1296y^{20}]x^{16}:$$

By using Table 2, we get

$$DM_1^*(G) = [384x^{24} + 44x^{20} + 40x^{16} + 41x^{17}]y^{24} + [32y^{16} + 33y^{17} + 36y^{20}]x^{16}|_{x=y=1} = 610,$$

$$DF^*(G) = [9216x^{24} + 976x^{20} + 832x^{16} + 865x^{17}]y^{24} + [512y^{16} + 545y^{17} + 656y^{20}]x^{16}|_{x=y=1} = 13602,$$

$$DM_2(G) = [4608x^{24} + 480x^{20} + 384x^{16} + 408x^{17}]y^{24} + [256y^{16} + 272y^{17} + 320y^{20}]x^{16}|_{x=y=1} = 6728,$$

$$DH(G) = [18432x^{24} + 1936x^{20} + 1600x^{16} + 1681x^{17}]y^{24} + [1024y^{16} + 1089y^{17} + 1296y^{20}]x^{16}|_{x=y=1} = 27058:$$

For γ -domination indices we have,

$$\varphi_\gamma(G, x, y) = 2y^6 + y^5 + 4y^4 + y^2 + [y^4 + y^5]x + 2x^2y^4 + [y^5 + y^6]x^4:$$

Then

$$(D_x + D_y)(\varphi_\gamma(G, x, y)) = 12y^6 + 5y^5 + 16y^4 + 2y^2 + [5y^4 + 6y^5]x + 12x^2y^4 + [9y^5 + 10y^6]x^4,$$

$$(D_x^2 + D_y^2)(\varphi_\gamma(G, x, y)) = 72y^6 + 25y^5 + 64y^4 + 4y^2 + [17y^4 + 26y^5]x + 40x^2y^4 + [41y^5 + 52y^6]x^4,$$

$$(D_x D_y)(\varphi_\gamma(G, x, y)) = [4y^4 + 5y^5]x + 16x^2y^4 + [20y^5 + 24y^6]x^4,$$

$$(D_x + D_y)^2(\varphi_\gamma(G, x, y)) = 72y^6 + 25y^5 + 64y^4 + 4y^2 + [25y^4 + 36y^5]x + 72x^2y^4 + [81y^5 + 100y^6]x^4.$$

By using Table 2, we get

$$\gamma M_1^*(G) = 12y^6 + 5y^5 + 16y^4 + 2y^2 + [5y^4 + 6y^5]x + 12x^2y^4 + [9y^5 + 10y^6]x^4|_{x=y=1} = 77,$$

$$\gamma F^*(G) = 72y^6 + 25y^5 + 64y^4 + 4y^2 + [17y^4 + 26y^5]x + 40x^2y^4 + [41y^5 + 52y^6]x^4|_{x=y=1} = 341,$$

$$\begin{aligned} {}_{\gamma}M_2(G) &= [4y^4 + 5y^5]x + 16x^2y^4 + [20y^5 + 24y^6]x^4 \Big|_{x=y=1} \\ &= 69, \end{aligned}$$

$$\begin{aligned} {}_{\gamma}H(G) &= 72y^6 + 25y^5 + 64y^4 + 4y^2 + [25y^4 + 36y^5]x \\ &+ 72x^2y^4 + [81y^5 + 100y^6]x^4 \Big|_{x=y=1} = 479; \end{aligned}$$

Clearly, $DM_1(G) = 6961$, ${}_{\gamma}M_1(G) = 119$, $DF(G) = 159345$, ${}_{\gamma}F(G) = 542$. ■

Theorem 2.4. Suppose H is the molecular graph of carbidopa, then

$$\varphi_d(H,x,y) = [10x^{48} + x^{40}]y^{48} + [2y^{48} + 2y^{32} + y^{40}]x^{32},$$

$$\begin{aligned} \varphi_y \\ (H,x,y) &= y^4 + [2 + 2x^4]y^6 + [1 + x^3]y^7 + [2 + 2x^2 + x^4 + x^7]y^8 \\ &+ [2 + x^8]y^{10}. \end{aligned}$$

Proof. Case1: Let

$$d_d m_{ij}(H) = |\{e = uv : d_d(u) = i, d_d(v) = j\}|.$$

The edge set of H can be divided into ve partitions based on the domination degree of end vertices of each edge as given in Table 5:

Hence,

$$\varphi_d(H,x,y) = [10x^{48} + x^{40}]y^{48} + [2y^{48} + 2y^{32} + y^{40}]x^{32},$$

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

TABLE 5 Edges partition

D_dm_{ij}	(48,48)	(32,48)	(33,32)	(32,40)	(40,48)
Number of edges	10	2	2	1	1

TABLE 6 Edge partition

d_ym_{ij}	(0,4)	(0,6)	(0,7)	(0,8)	(0,10)	(2,8)	(3,7)	(4,6)	(8,10)	(4,8)	(7,8)
Number of edges	1	2	1	2	2	2	1	2	1	1	1

Hence

$$\begin{aligned} \varphi_y(H,x,y) &= y^4 + [2 + 2x^4]y^6 + [1 + x^3]y^7 + [2 + 2x^2 + x^4 + x^7] \\ &y^8 + [2 + x^8]y^{10}. \end{aligned}$$

Theorem 2.5. Suppose H is the molecular graph of carbidopa. Then

1. $DM_1^*(H) = 1408$, ${}_{\gamma}M_1^*(H) = 154$,

2. $DF^*(H) = 63360$, ${}_{\gamma}F^*(H) = 1120$,

3. $DM_2(H) = 31360$, ${}_{\gamma}M_2(H) = 269$,

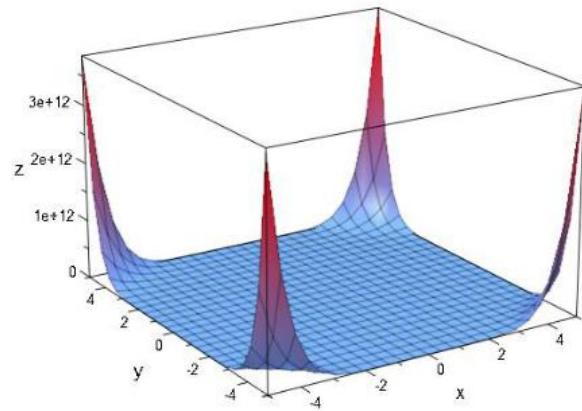
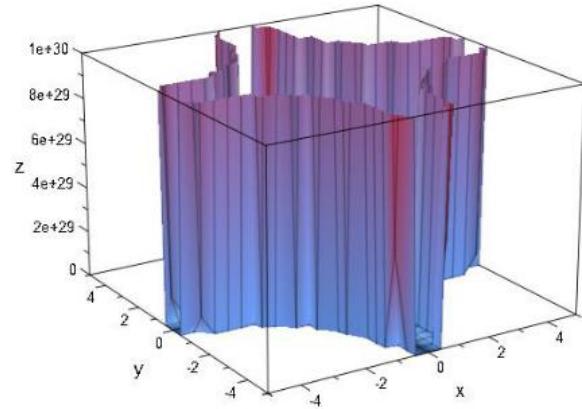


FIGURE 4 Plotting of (a) φ_d -polynomial and (b) φ_y -polynomial of Carbidopa

4. $DH(H) = 126080$, ${}_{\gamma}H(H) = 1658$,

5. $DM_1(H) = 32320$, ${}_{\gamma}M_1(H) = 396$,

6. $DF(H) = 1489408$, ${}_{\gamma}F(H) = 2970$:

Proof. We have,

$$\varphi_d(H,x,y) = [10x^{48} + x^{40}]y^{48} + [2y^{48} + 2y^{32} + y^{40}]x^{32}.$$

Then

$$(D_x + D_y)(\varphi_d(H, x, y)) = [960x^{48} + 88x^{40}]y^{48} + [160y^{48} + 128y^{32} + 72y^{40}]x^{32},$$

$$(D_x^2 + D_y^2)(\varphi_d(H, x, y)) = [46080x^{48} + 3904x^{40}]y^{48} + [6656y^{48} + 4096y^{32} + 2624y^{40}]x^{32},$$

$$(D_x D_y)(\varphi_d(H, x, y)) = [23040x^{48} + 1920x^{40}]y^{48} + [3072y^{48} + 2048y^{32} + 1280y^{40}]x^{32},$$

$$(D_x + D_y)^2(\varphi_d(H, x, y)) = [92160x^{48} + 7744x^{40}]y^{48} + [12800y^{48} + 8192y^{32} + 5184y^{40}]x^{32};$$

By using Table 2, we get

$$DM_1^*(H) = [960x^{48} + 88x^{40}]y^{48} + [160y^{48} + 128y^{32} + 72y^{40}]x^{32} \Big|_{x=y=1} = 1408,$$

$$DF^*(H) = [46080x^{48} + 3904x^{40}]y^{48} + [6656y^{48} + 4096y^{32} + 2624y^{40}]x^{32} \Big|_{x=y=1} = 63360,$$

$$DM_2(H) = [23040x^{48} + 1920x^{40}]y^{48} + [3072y^{48} + 2048y^{32} + 1280y^{40}]x^{32} \Big|_{x=y=1} = 31360,$$

$$DH(H) = [92160x^{48} + 7744x^{40}]y^{48} + [12800y^{48} + 8192y^{32} + 5184y^{40}]x^{32} \Big|_{x=y=1} = 126080.$$

For γ -domination indices we have,

$$\varphi_\gamma(H, x, y) = y^4 + [2 + 2x^4]y^6 + [1 + x^2]y^7 + [2 + 2x^2 + x^4 + x^7]y^8 + [2 + x^8]y^{10}.$$

Then

$$(D_x + D_y)(\varphi_\gamma(H, x, y)) = 4y^4 + [12 + 20x^4]y^6 + [7 + 10x^3]y^7 + [16 + 20x^2 + 12x^4 + 15x^7]y^8 + [20 + 18x^8]y^{10},$$

$$(D_x^2 + D_y^2)(\varphi_\gamma(H, x, y)) = 16y^4 + [72 + 104x^4]y^6 + [49 + 8x^3]y^7 + [128 + 136x^2 + 80x^4 + 113x^7]y^8 + [200 + 164x^8]y^{10},$$

$$(D_x D_y)(\varphi_\gamma(H, x, y)) = 48x^4y^6 + 21x^3y^7 + [32x^2 + 32x^4 + 56x^7]y^8 + 80x^8y^{10},$$

$$(D_x + D_y)^2(\varphi_\gamma(H, x, y)) = 16y^4 + [72 + 200x^4]y^6 + [49 + 100x^3]y^7 + [128 + 200x^2 + 144x^4 + 225x^7]y^8 + [200 + 324x^8]y^{10};$$

By using Table 2, we get

$$M_1^*(H) = 4y^4 + [12 + 20x^4]y^6 + [7 + 10x^3]y^7 + [16 + 20x^2 + 12x^4 + 15x^7]y^8 + [20 + 18x^8]y^{10} \Big|_{x=y=1} = 154,$$

$$F^*(H) = 16y^4 + [72 + 104x^4]y^6 + [49 + 58x^3]y^7 + [128 + 136x^2 + 80x^4 + 113x^7]y^8 + [200 + 164x^8]y^{10} \Big|_{x=y=1} = 1120,$$

$$M_2(H) = 48x^4y^6 + 21x^3y^7 + [32x^2 + 32x^4 + 56x^7]y^8 + 80x^8y^{10} \Big|_{x=y=1} = 269,$$

$$H(G) = 16y^4 + [72 + 200x^4]y^6 + [49 + 100x^3]y^7 + [128 + 200x^2 + 144x^4 + 225x^7]y^8 + [200 + 324x^8]y^{10} \Big|_{x=y=1} = 1658;$$

Clearly, $DM_1(G) = 32320$, $\gamma M_1(G) = 396$, $DF(G) = 1489408$, $\gamma F(G) = 2970$. ■

Conclusion

We have studied and computed the properties of Carbidopa-Levodopa used for treatment Parkinson's disease through domination and γ -Domination topological indices. First, we found φ_d polynomial and φ_γ polynomial and their respective 3D graphs (Figures 3 and 4). Then we computed the domination and γ -Domination indices from these polynomials.

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