

**Original Research Article****M-Polynomials and Topological Indices of Porphyrin-Cored Dendrimers**

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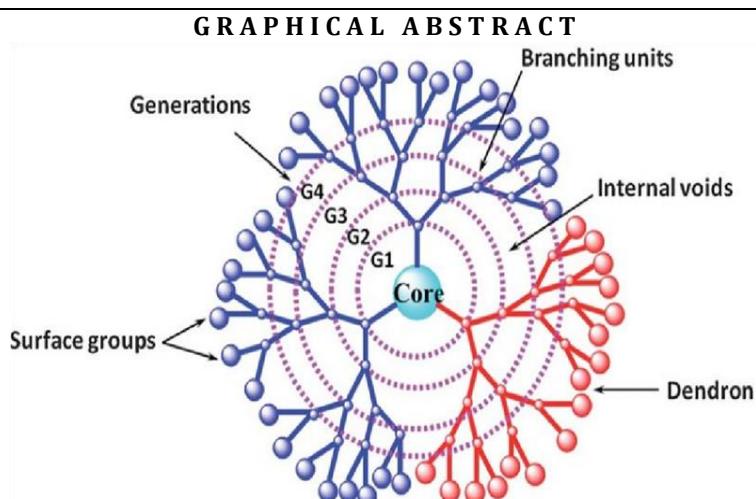
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Molecular structure

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**ABSTRACT**

Porphyrin-cored dendrimers of the  $G_n$  generation with  $n \geq 1$  are of four types *PCD-I*, *PCD-II*, *PCD-III*, and *PCD-IV*. In this article, several necessary chemical structures of porphyrin-cored dendrimers are considered. Also, their M-Polynomials are calculated using the partition of the edges. By applying these M-polynomials to porphyrin-cored dendrimers, some important topological indices are computed. Finally, the results are taken from Maple 2022 to see the dependency concerning the involved structural parameters. Our results will help researchers to observe the strong correlation between the physicochemical properties of dendrimers and topological indices in the pharmaceutical industry and drug delivery.



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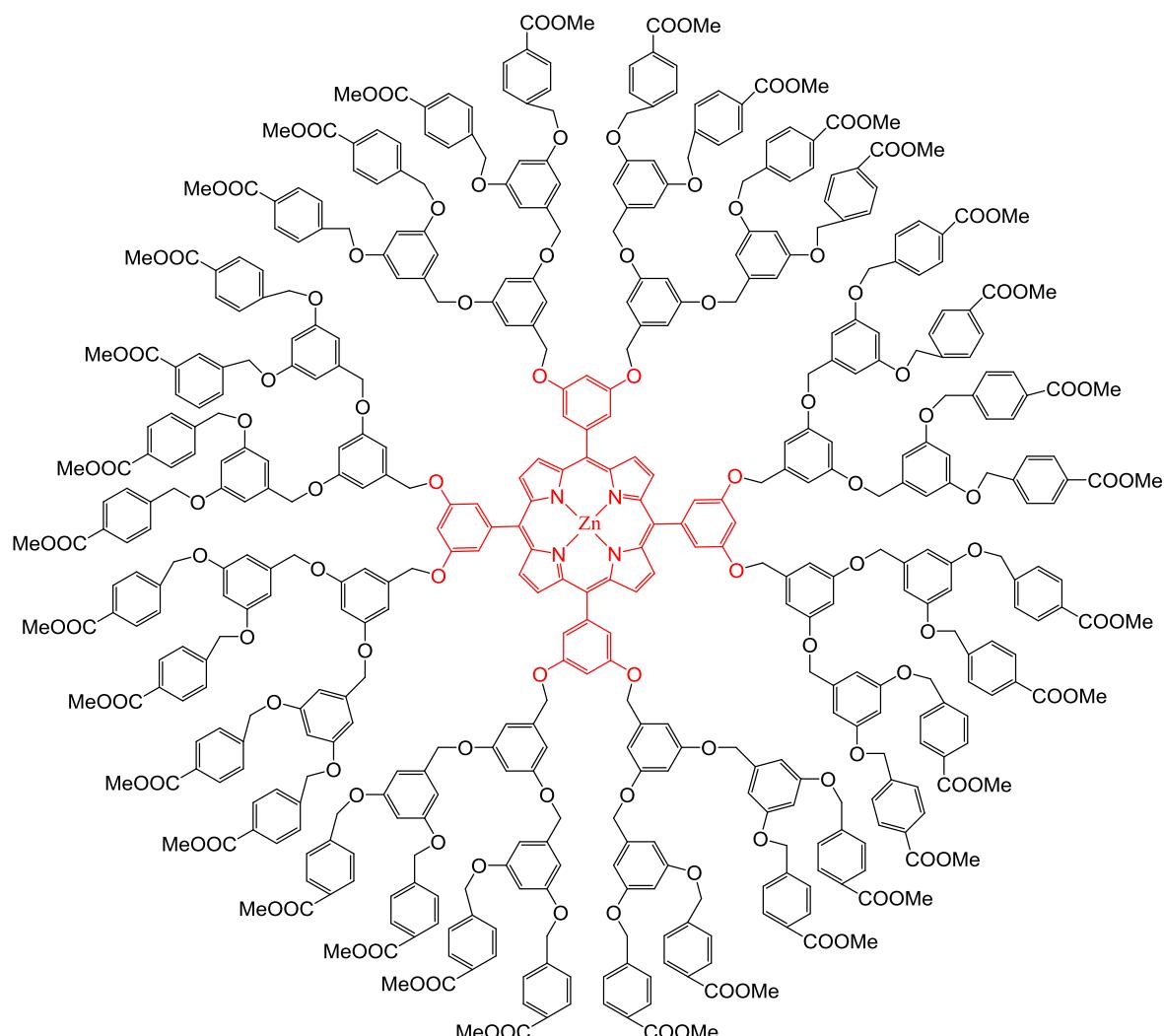
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## Introduction

Dendrimers are multi-branched macromolecules of nanometric size. Dendrimers consist of three distinct elements as a central core and an inner surface with a dendritic structure consisting of branches, with external surface groups, see **Figure 1** [1]. There is a powerful exclusivity among the molecular structures of chemical compounds and their chemical properties. Topological indices which are also called molecular descriptors are numerical quantities associated with a graph used to predict the physicochemical features of chemical structures such as melting, boiling, flash points, enthalpy of vaporization, etc. [2, 3]. Among algebraic Polynomials, M-Polynomial was expressed by Klavzar and Deutsch [4] and has a fundamental role in specifying the formula of topological indices based on the degree [5]. M-

polynomial helps to find several topological indices based on the degree, such as the first and second Zagreb, modified second Zagreb [6], symmetric division [7], generalized Randić [8], inverse Randić inverse sum [8], harmonic, and augmented Zagreb indices [4, 9]. In primary definitions, see [10, 11]. **Table 1** presents some topological indices based on the degree derived from M-polynomial [4, 12]. Throughout this article, all graphs are simple and connected. We denote the degree of the vertex  $v$  with  $d(v)$ , the vertices, and edges set of graph  $G$  with  $V(G)$  and  $E(G)$  respectively, and the number of edges in  $G$  with  $e(G)$ . Likewise, we use the following formula, which is well known as the degree-sum formula [13].

$$\sum d(v) = 2e(G)$$



**Figure 1:** Dendrimer with porphyrin core functionalized with Fréchet-type dendrons

## Materials and Methods

In this article, M-polynomials of Porphyrin-cored dendrimers of the  $G_n$  generation of the first, second, third, and fourth type are calculated. Using these M-Polynomials, several topological indices based on the obtained degree. Combinatorial computations with the technique of counting the degree of vertices and the method of partition edges have been applied to obtain the results. Then, using these partitions, the form of the M-polynomial of Porphyrin-cored dendrimers is obtained. Furthermore, the surface of the M-polynomial is plotted using Maple 2022.

**Definition 1** [5]. A loop is an edge whose terminal vertices are equal. Multiple edges are edges with the same terminal vertices. A simple graph does not have loops and multiple edges.

**Definition 2** [5]. A graph G is Connected, whenever there is a path among both vertices.

**Definition 3** [5]. The M-polynomial of graph G is introduced as follows:

$$M(G; x, y) = \sum_{i \leq j} m_{ij} x^i y^j$$

Such that

$$m_{ij} = \{uv \in E(G) \mid d_u = i, d_v = j\}$$

**Table 1:** Topological indices based on the degree derived from M-Polynomial

Topological indices	Derivation from $M(G, x, y) = f(x, y)$
The First Zagreb $M_1(G)$	$(D_x + D_y)(f(x, y)) _{x=y=1}$
The Second Zagreb $M_2(G)$	$(D_x D_y)(f(x, y)) _{x=y=1}$
The Second Modified Zagreb ${}^m M_2(G)$	$(S_x S_y)(f(x, y)) _{x=y=1}$
Inverse Randić $RR_\alpha(G)$	$(D_x^\alpha D_y^\alpha)(f(x, y)) _{x=y=1}$
General Randić $R_\alpha(G)$	$(S_x^\alpha S_y^\alpha)(f(x, y)) _{x=y=1}$
Symmetric Division $SSD(G)$	$(D_x S_y + S_x D_y)(f(x, y)) _{x=y=1}$
Harmonic $H(G)$	$(2S_x J)(f(x, y)) _{x=1}$
Inverse sum $I(G)$	$(S_x J D_x D_y)(f(x, y)) _{x=1}$
Augmented Zagreb $A(G)$	$(S_x^3 Q_{-2} J D_x^3 D_y^3)(f(x, y)) _{x=1}$

$$D_x = x \frac{\partial f(x,y)}{\partial x}, D_y = y \frac{\partial f(x,y)}{\partial y}, S_x = \int_0^x \frac{f(t,y)}{t} d(t), S_y = \int_0^y \frac{f(x,t)}{t} d(t)$$

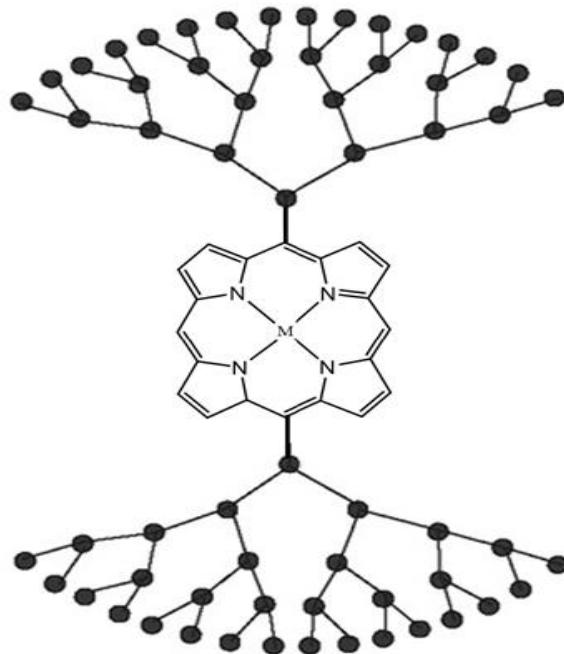
$$Jf(x,y) = f(x,x), Q_\alpha = x^\alpha f(x,y) \quad (\alpha \neq 0)$$

## Results and Discussion

### Porphyrin-cored dendrimer- I (PCD-I)

Our first molecular diagram is PCD-I of generation  $G_n$  with  $n \geq 1$  growth stage [3]. The PCD-I is

composed of 2 branches, with one core at its centre. The central core comprises 25 vertex and 34 edges, as depicted in Figure 2. According to Table 2 and by degree-sum formula, the total number of edges in PCD-I is  $4 \times 2^n + 30$  [3].

**Figure 2:** The molecular diagram of Porphyrin-cored dendrimer *PCD-I***Table 2:** The vertices partitions of PCD-I

Degree of the vertex	Central core	In one of the branches	Total number of vertices
1	-	$2^n$	$2^{n+1}$
2	10	-	10
3	14	$2^n - 1$	$2^{n+1} + 12$
4	1	-	1
Total number of vertices	25	$2^{n+1} - 1$	$2^{n+2} + 23$

In [Figure 3](#), according to the degrees of vertices incident with each edge, a set of edges *PCD-I* can be partitioned into 5 categories. We compute their cardinalities in [Table 3](#).

$$\begin{aligned} E(2,3) &= \{uv \in E(PCD-I) \mid d_u = 2, d_v = 3\}, \\ E(3,3) &= \{uv \in E(PCD-I) \mid d_u = 3, d_v = 3\}, \\ E(3,4) &= \{uv \in E(PCD-I) \mid d_u = 3, d_v = 4\}. \end{aligned}$$

$$E(1,3) = \{uv \in E(PCD-I) \mid d_u = 1, d_v = 3\},$$

$$E(2,2) = \{uv \in E(PCD-I) \mid d_u = 2, d_v = 2\},$$

**Table 3:** The edges partitions of PCD-I

$E(i, j)$	Number of edges
$E(1,3)$	$2^{n+1}$
$E(2,2)$	4
$E(2,3)$	12
$E(3,3)$	$2^{n+1} + 10$
$E(3,4)$	4

**Theorem 1.** Suppose  $M(PCD-I; x, y)$  be  $M$ -Polynomial of PCD-I. Then, we have:

$$M(PCD-I; x, y) = 2^{n+1}xy^3 + 4x^2y^2 + 12x^2y^3 + (2^{n+1} + 10)x^3y^3 + 4x^3y^4.$$

**Proof.** From the vertices and edges partition of  $PCD-I$  given in Tables 2 and 3, and using Definition 3, we have:

$$\begin{aligned} M(PCD-I; x, y) &= \sum_{i \leq j} m_{ij} x^i y^j \\ &= \sum_{uv \in E(1,3)} m_{13} x^1 y^3 + \sum_{uv \in E(2,2)} m_{22} x^2 y^2 + \sum_{uv \in E(2,3)} m_{23} x^2 y^3 + \sum_{uv \in E(3,3)} m_{33} x^3 y^3 + \sum_{uv \in E(3,4)} m_{34} x^3 y^4 \\ &= |E(1,3)|x^1 y^3 + |E(2,2)|x^2 y^2 + |E(2,3)|x^2 y^3 + |E(3,3)|x^3 y^3 + |E(3,4)|x^3 y^4 \\ &= 2^{n+1}xy^3 + 4x^2y^2 + 12x^2y^3 + (2^{n+1} + 10)x^3y^3 + 4x^3y^4. \end{aligned}$$

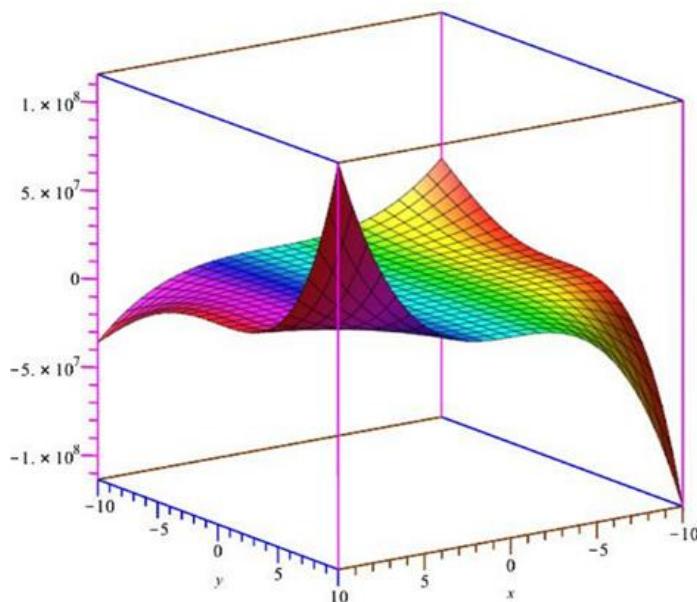


Figure 3: Plot of M-Polynomial PCD-I of generation  $G_3$

**Proposition 2.** Let  $PCD-I$  be a molecule graph of generation  $G_n$  with  $n \geq 1$  growth stag. Then,

$$(1) \quad M_1(PCD-I) = 12(2^{n+1}) + 164,$$

$$(2) \quad M_2(PCD-I) = 12(2^{n+1}) + 226,$$

$$(3) \quad {}^m M_2(PCD-I) = \frac{4}{9}(2^{n+1}) + \frac{41}{9},$$

$$(4) \quad R_\alpha(PCD-I) = 3^\alpha(2^{n+1}) + 4^{\alpha+1} + 6^\alpha(12) + 9^\alpha(2^{n+1} + 10) + 12^\alpha(4),$$

$$(5) \quad RR_{\alpha}(PCD-I) = \frac{1}{3^{\alpha}}(2^{n+1}) + \frac{1}{4^{\alpha-1}} + \frac{1}{6^{\alpha}}(12) + \frac{1}{9^{\alpha}}(2^{n+1}+10),$$

$$(6) \quad SSD(PCD-I) = \frac{14}{3}(2^{n+1}) + \frac{170}{3},$$

$$(7) \quad H(PCD-I) = \frac{5}{6}(2^{n+1}) + \frac{152}{15},$$

$$(8) \quad I(PCD-I) = \frac{9}{4}(2^{n+1}) + \frac{1409}{35},$$

$$(9) \quad A(PCD-I) = \frac{945}{64}(2^{n+1}) + \frac{2377618}{8000}.$$

**Proof.** Let  $f(x,y)=2^{n+1}xy^3+4x^2y^2+12x^2y^3+(2^{n+1}+10)x^3y^3+4x^3y^4$ .

Then,

$$D_x(f(x,y))=3(2^{n+1})xy^3+8x^2y^2+24x^2y^3+3(2^{n+1}+10)x^3y^3+12x^3y^4,$$

$$D_y(f(x,y))=3(2^{n+1})xy^3+8x^2y^2+36x^2y^3+3(2^{n+1}+10)x^3y^3+16x^3y^4,$$

$$D_xD_y(f(x,y))=3(2^{n+1})xy^3+16x^2y^2+72x^2y^3+9(2^{n+1}+10)x^3y^3+48x^3y^4,$$

$$S_x(f(x,y))=2^{n+1}xy^3+2x^2y^2+6x^2y^3+\frac{1}{3}(2^{n+1}+10)x^3y^3+\frac{4}{3}x^3y^4,$$

$$S_y(f(x,y))=\frac{2^{n+1}}{3}xy^3+2x^2y^2+4x^2y^3+\frac{1}{3}(2^{n+1}+10)x^3y^3+\frac{4}{3}x^3y^4,$$

$$S_xS_y(f(x,y))=\frac{2^{n+1}}{3}xy^3+x^2y^2+2x^2y^3+\frac{1}{9}(2^{n+1}+14)x^3y^3,$$

$$D_xS_y(f(x,y))=\frac{2^{n+1}}{3}xy^3+4x^2y^2+(2^{n+1}+18)x^2y^3+4x^3y^3,$$

$$S_xD_y(f(x,y))=3(2^{n+1})xy^3+4x^2y^2+18x^2y^3+\frac{(2^{n+1}+26)}{3}x^3y^3,$$

$$S_xJD_xD_y(f(x,y))=\frac{19}{4}(2^{n+1})x^4+\frac{72}{5}x^5+\frac{3}{2}(2^{n+1}+10)x^6+\frac{48}{7}x^7,$$

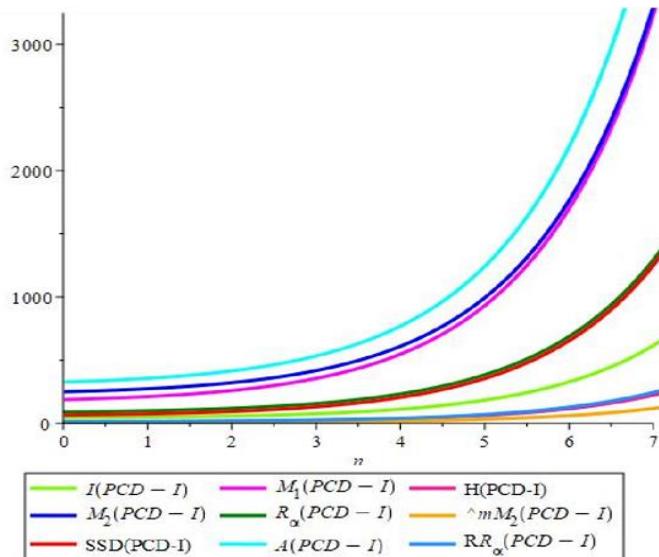
$$D_x^{\alpha}D_y^{\alpha}(f(x,y))=3^{\alpha}(2^{n+1})xy^3+4^{\alpha+1}x^2y^2+12(6^{\alpha})x^2y^3 \\ +9(2^{n+1}+10)x^3y^3+4(12^{\alpha})x^3y^4,$$

$$S_x^{\alpha}S_y^{\alpha}(f(x,y))=\frac{2^{n+1}}{3^{\alpha}}x^1y^3+(\frac{1}{4})^{\alpha-1}x^2y^2+12(\frac{1}{6^{\alpha}})x^2y^3$$

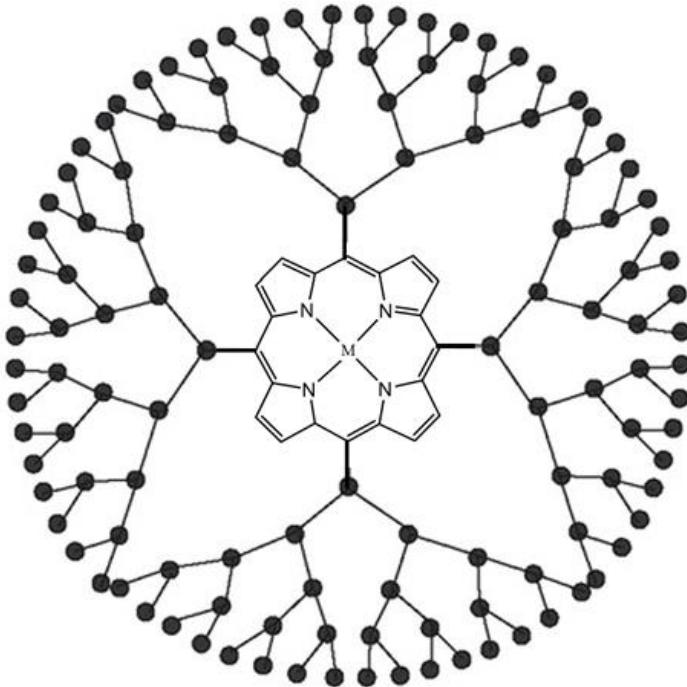
$$+(\frac{1}{9})^\alpha (2^{n+1} + 14)x^3y^3,$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3 (f(x, y)) = (\frac{27}{8} \times 2^{n+1} + 32)x^2 + 96x^3 + \frac{729}{64}(2^{n+1} + 10)x^4 \\ + \frac{6912}{125}x^5.$$

Now, using [Table 1](#), the proof is complete.



**Figure 4:** Plot of comparison topological indices of PCD-I



**Figure 5:** The molecular diagram of Porphyrin-cored dendrimer PCD-II

**Table 4:** The vertices partitions of PCD-II

Degree of the vertex	Central core	In one of the branches	Total number of vertices
1	-	$2^n$	$2^{n+2}$
2	8	-	8
3	16	$2^n - 1$	$2^{n+2} + 12$
4	1	-	1
Total number of vertices	25	$2^{n+1} - 1$	$2^{n+3} + 21$

*Porphyrin-cored dendrimer-II (PCD-II)*

Our second molecular diagram is PCD-II of generation  $G_n$  with  $n \geq 1$  growth stage. PCD-II is composed of four similar branches, such that one core is at its center. The central core is composed of 25 vertex and 36 edges, as displayed in [Figure 5](#). According to [Table 4](#) and by degree-sum formula, the total number of edges in PCD-II is  $8 \times 2^n + 28$  [3].

In [Figure 5](#), according to degrees of the vertex incident with each edge, set of edges PCD-II can

be partitioned into 5 categories. We compute their cardinalities in [Table 5](#).

$$\begin{aligned} E(1,3) &= \{uv \in E(PCD-II) \mid d_u = 1, d_v = 3\}, \\ E(2,2) &= \{uv \in E(PCD-II) \mid d_u = 2, d_v = 2\}, \\ E(2,3) &= \{uv \in E(PCD-II) \mid d_u = 2, d_v = 3\}, \\ E(3,3) &= \{uv \in E(PCD-II) \mid d_u = 3, d_v = 3\}, \\ E(3,4) &= \{uv \in E(PCD-II) \mid d_u = 3, d_v = 4\}. \end{aligned}$$

**Table 5:** The edges partitions of PCD-II

$E(i, j)$	Number of edges
$E(1,3)$	$2^{n+2}$
$E(2,2)$	4
$E(2,3)$	8
$E(3,3)$	$2^{n+2} + 12$
$E(3,4)$	4

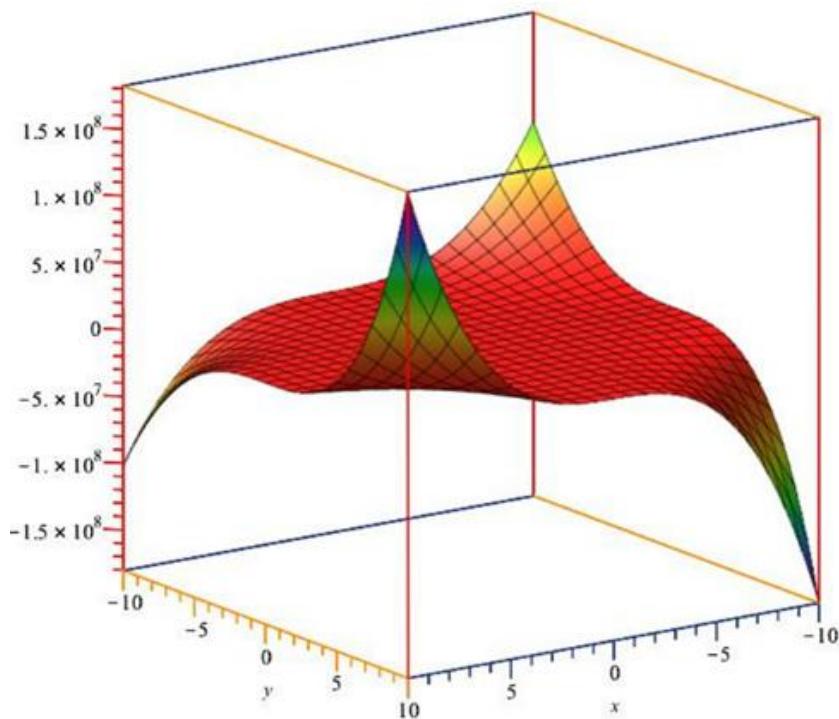
**Theorem 3.** Suppose  $M(PCD-II; x, y)$  be M-Polynomial of PCD-II. Then, we have:

$$M(PCD-II; x, y) = (2^{n+2})xy^3 + 4x^2y^2 + 8x^2y^3 + (2^{n+2} + 12)x^3y^3 + 4x^3y^4.$$

**Proof.** From the edges partition of PCD-II given in [Table 3](#) and using Definition 3, we have:

$$\begin{aligned} M(PCD-II; x, y) &= \sum_{i \leq j} m_{ij} x^i y^j \\ &= \sum_{uv \in E(1,3)} m_{13} x^1 y^3 + \sum_{uv \in E(2,2)} m_{22} x^2 y^2 + \sum_{uv \in E(2,3)} m_{23} x^2 y^3 + \sum_{uv \in E(3,3)} m_{33} x^3 y^3 + \sum_{uv \in E(3,4)} m_{34} x^3 y^4. \\ &= |E(1,3)|x^1 y^3 + |E(2,2)|x^2 y^2 + |E(2,3)|x^2 y^3 + |E(3,3)|x^3 y^3 + |E(3,4)|x^3 y^4 \end{aligned}$$

$$= (2^{n+2})xy^3 + 4x^2y^2 + 8x^2y^3 + (2^{n+2} + 12)x^3y^3 + 4x^3y^4.$$



**Figure 6:** Plot of M-Polynomial PCD-II graph of generation  $G_3$

**Proposition 4.** Let PCD-II be a molecule graph of generation  $G_n$  with  $n \geq 1$  growth stage. Then,

$$(1) \quad M_1(PCD-II) = 40(2^n) + 156,$$

$$(2) \quad M_2(PCD-II) = 48(2^n) + 220,$$

$$(3) \quad {}^mM_2(PCD-II) = \frac{4}{3}(2^n) + \frac{46}{9},$$

$$(4) \quad R_\alpha(PCD-II) = 3^\alpha(4)(2^n) + 4^{\alpha+1} + 6^\alpha(8) + 9^\alpha(4 \times 2^n + 12) + 12^\alpha(4),$$

$$(5) \quad RR_\alpha(PCD-II) = \frac{1}{3^\alpha}(4)(2^n) + \frac{1}{4^{\alpha-1}} + \frac{1}{6^\alpha}(8) + \frac{1}{12^{\alpha-1}} + \frac{1}{9^\alpha}(4 \times 2^n + 12),$$

$$(6) \quad SSD(PCD-II) = \frac{64}{3}(2^n) + \frac{191}{3},$$

$$(7) \quad H(PCD-II) = \frac{10}{3}(2^n) + \frac{362}{35},$$

$$(8) \quad I(PCD-II) = 9(2^n) + \frac{1346}{35},$$

$$(9) \quad A(PCD-II) = \frac{945}{16}(2^n) + \frac{575967}{2000}.$$

**Proof.** Let  $f(x, y) = (2^{n+2})xy^3 + 4x^2y^2 + 8x^2y^3 + (2^{n+2} + 12)x^3y^3 + 4x^3y^4$ ,

Then,

$$D_x(f(x, y)) = (2^{n+2})xy^3 + 8x^2y^2 + 16x^2y^3 + 3(2^{n+2} + 12)x^3y^3 + 12x^3y^4,$$

$$D_y(f(x, y)) = 3(2^{n+2})xy^3 + 8x^2y^2 + 24x^2y^3 + 3(2^{n+2} + 12)x^3y^3 + 16x^3y^4,$$

$$D_x D_y(f(x, y)) = 3(2^{n+2})xy^3 + 16x^2y^2 + 48x^2y^3 + 9(2^{n+2} + 12)x^3y^3 + 48x^3y^4,$$

$$S_x(f(x, y)) = 2^{n+2}xy^3 + 2x^2y^2 + 4x^2y^3 + \frac{1}{3}(2^{n+2} + 12)x^3y^3 + \frac{4}{3}x^3y^4,$$

$$S_y(f(x, y)) = \frac{1}{3}(2^{n+2})xy^3 + 2x^2y^2 + \frac{8}{3}x^2y^3 + \frac{1}{3}(2^{n+2} + 12)x^3y^3 + 3x^3y^4,$$

$$S_x S_y(f(x, y)) = \frac{1}{3}(2^{n+2})xy^3 + x^2y^2 + \frac{4}{3}x^2y^3 + \frac{1}{9}(2^{n+2} + 12)x^3y^3 + x^3y^4,$$

$$D_x S_y(f(x, y)) = \frac{1}{3}(2^{n+2})xy^3 + 4x^2y^2 + \frac{16}{3}x^2y^3 + (2^{n+2} + 12)x^3y^3 + 9x^3y^4,$$

$$S_x D_y(f(x, y)) = 3(2^{n+2})xy^3 + 4x^2y^2 + 12x^2y^3 + (2^{n+2} + 12)x^3y^3 + \frac{16}{3}x^3y^4,$$

$$S_x J D_x D_y(f(x, y)) = (3 \times 2^n + 4)x^4 + \frac{48}{5}x^5 + 6(2^n + 3)x^6 + \frac{48}{7}x^7,$$

$$D_x^\alpha D_y^\alpha(f(x, y)) = 4(3^\alpha)(2^n)x^1y^3 + 4^{\alpha+1}x^2y^2 + 8(6^\alpha)x^2y^3 + 9^\alpha(2^{n+2} + 12)x^3y^3$$

$$+ 4(12^\alpha)x^3y^3,$$

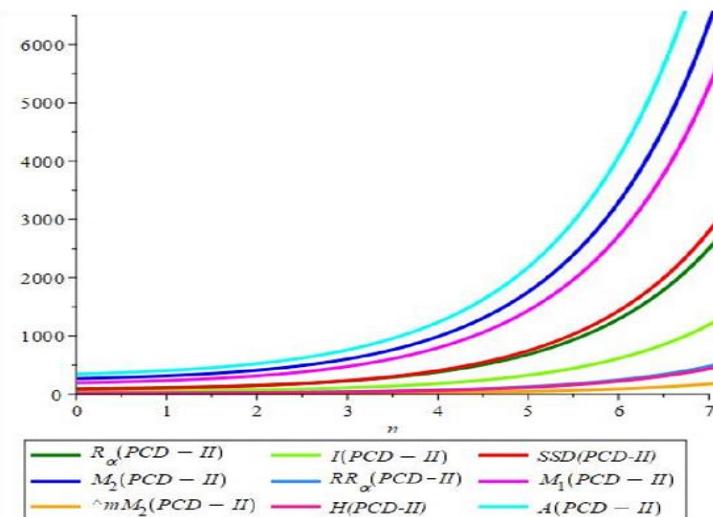
$$S_x^\alpha S_y^\alpha(f(x, y)) = (\frac{1}{3})^\alpha(2^{n+2})x^1y^3 + (\frac{1}{4})^{\alpha-1}x^2y^2 + 8(\frac{1}{6})^\alpha x^2y^3 + \frac{(2^{n+2} + 12)}{9^\alpha}x^3y^3$$

$$+ (\frac{1}{12})^{\alpha-1}x^3y^4,$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) = (\frac{27}{8} \times 2^{n+1} + 32)x^2 + 96x^3 + \frac{729}{64}(2^{n+1} + 10)x^4$$

$$+ \frac{6912}{125}x^5,$$

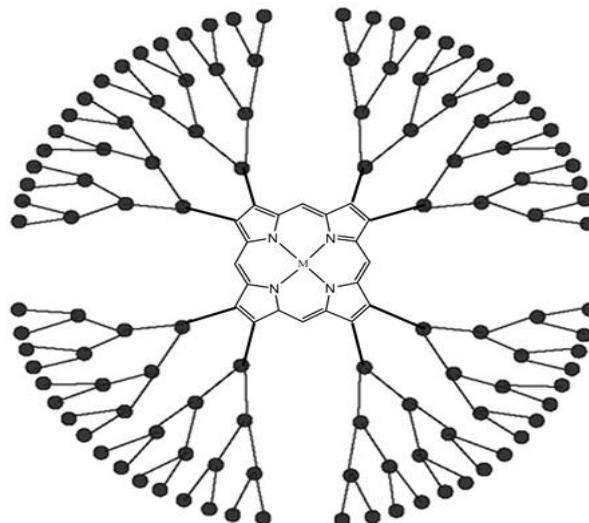
Now, using [Table 1](#), the proof is complete.

**Figure 7:** Plot of comparison topological indices of PCD-II

### Porphyrin-cored dendrimer- III (PCD-III)

Our third molecular diagram is *PCD-III* of generation  $G_n$  with  $n \geq 1$  growth stage. *PCD-III* is composed of 25 vertex and eight similar branches, such that one core is at its center, as demonstrated

in [Figure 8](#). The central core is composed of 25 vertices and 40 edges, as illustrated in [Figure 8](#). According to [Table 6](#) and by degree-sum formula, the total number of edges in *PCD-III* is  $16 \times 2^n + 24$  [3].

**Figure 8:** The molecular diagram of Porphyrin-cored dendrimer *PCD-III***Table 6:** The vertices partitions of PCD-III

Degree of the vertex	Central core	In one of the branches	Total number of vertices
1	-	$2^n$	$12 \times 2^n$
2	-	-	-
3	24	$2^n - 1$	$12 \times 2^n + 12$
4	1	-	1
Total number of vertices	25	$2^{n+1} - 1$	$24 \times 2^n + 13$

In [Figure 8](#), according to the degrees of the vertex incident with each edge, a set of edges *PCD-III* can

be partitioned into 4 categories. We compute their cardinalities in [Table 7](#).

$$\begin{aligned} E(3,3) &= \{uv \in E(PCD-III) \mid d_u = 3, d_v = 3\}, \\ E(1,3) &= \{uv \in E(PCD-III) \mid d_u = 1, d_v = 3\}, \quad E(3,4) = \{uv \in E(PCD-III) \mid d_u = 3, d_v = 4\}. \\ E(2,3) &= \{uv \in E(PCD-III) \mid d_u = 2, d_v = 3\}, \end{aligned}$$

**Table 7:** The edges partitions of PCD - III

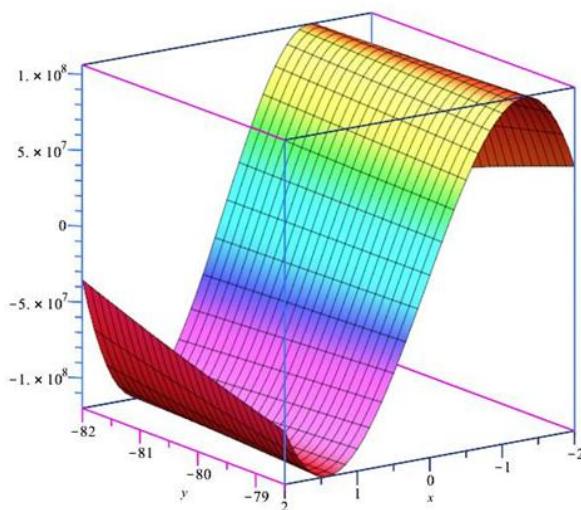
$E(i, j)$	Number of edges
$E(1,3)$	$2^{n+3}$
$E(2,3)$	8
$E(3,3)$	$2^{n+3} + 12$
$E(3,4)$	4

**Theorem 5.** Suppose  $M(PCD-III; x, y)$  be M-Polynomial of PCD-III. Then, we have:

$$M(PCD-III; x, y) = (2^{n+3})xy^3 + 8x^2y^3 + (2^{n+3} + 12)x^3y^3 + 4x^3y^4$$

**Proof.** From the edges partition of PCD - III given in Table 4 and using Definition 3, we have:

$$\begin{aligned} M(PCD-III; x, y) &= \sum_{i \leq j} m_{ij} x^i y^j \\ &= \sum_{uv \in E(1,3)} m_{13} x^1 y^3 + \sum_{uv \in E(2,3)} m_{23} x^2 y^3 + \sum_{uv \in E(3,3)} m_{33} x^3 y^3 + \sum_{uv \in E(3,4)} m_{34} x^3 y^4 \\ &\equiv |E(1,3)|x^1 y^3 + |E(2,3)|x^2 y^3 + |E(3,3)|x^3 y^3 + |E(3,4)|x^3 y^4 \\ &= (2^{n+3})xy^3 + 8x^2y^3 + (2^{n+3} + 12)x^3y^3 + 4x^3y^4. \end{aligned}$$

**Figure 9.** Plot of M-polynomial PCD-III of generation  $G_3$

**Proposition 6.** Let PCD-III be the Porphyrin-cored dendrimer of the third type of generation  $G_n$  with  $n \geq 1$  growth stage. Then,

$$(1) \quad M_1(PCD-III) = 80(2^n) + 140,$$

$$(2) \quad M_2(PCD-III) = 96(2^n) + 204,$$

$$(3) \quad {}^m M_2(PCD-III) = \frac{32}{9}(2^n) + 3,$$

$$(4) \quad R_\alpha(PCD-III) = 3^\alpha(2^{n+3}) + 6^\alpha(8) + 9^\alpha(2^{n+3} + 12) + 12^\alpha\left(\frac{1}{9}\right),$$

$$(5) \quad RR_\alpha(PCD-III) = \frac{1}{3^\alpha}(2^{n+3}) + \frac{1}{6^\alpha}(8) + \frac{1}{9^\alpha}(2^{n+3} + 12) + \frac{1}{12^\alpha}(4),$$

$$(6) \quad SSD(PCD-III) = \frac{128}{3}(2^n) + 653,$$

$$(7) \quad H(PCD-III) = \frac{20}{3}(2^n) + \frac{292}{35},$$

$$(8) \quad I(PCD-III) = 18(2^n) + \frac{1206}{35},$$

$$(9) \quad A(PCD-III) = \frac{945}{8}(2^n) + \frac{8192}{35}.$$

**Proof.** Let  $f(x, y) = (2^{n+3})xy^3 + 8x^2y^3 + (2^{n+3} + 12)x^3y^3 + 4x^3y^4$ ,

Then,

$$D_x(f(x, y)) = (2^{n+3})xy^3 + 16x^2y^3 + 3(2^{n+3} + 12)x^3y^3 + 12x^3y^4,$$

$$D_y(f(x, y)) = 3(2^{n+3})xy^3 + 24x^2y^3 + 3(2^{n+3} + 12)x^3y^3 + 16x^3y^4,$$

$$D_x D_y(f(x, y)) = 3(2^{n+3})xy^3 + 48x^2y^3 + 9(2^{n+3} + 12)x^3y^3 + 48x^3y^4,$$

$$S_x(f(x, y)) = 2^{n+3}xy^3 + 4x^2y^3 + \frac{1}{3}(2^{n+3} + 12)x^3y^3 + \frac{4}{3}x^3y^4,$$

$$S_y(f(x, y)) = \frac{1}{3}(2^{n+3})xy^3 + \frac{8}{3}x^2y^3 + \frac{1}{3}(2^{n+3} + 12)x^3y^3 + x^3y^4,$$

$$S_x S_y(f(x, y)) = \frac{1}{3}(2^{n+3})xy^3 + \frac{4}{3}x^2y^3 + \frac{1}{9}(2^{n+3} + 12)x^3y^3 + \frac{1}{3}x^3y^4,$$

$$D_x S_y(f(x, y)) = \frac{1}{3}(2^{n+3})xy^3 + \frac{16}{3}x^2y^3 + (2^{n+3} + 12)x^3y^3 + 3x^3y^4,$$

$$S_x D_y(f(x, y)) = 3(2^{n+3})xy^3 + 12x^2y^3 + (2^{n+3} + 12)x^3y^3 + \frac{16}{3}x^3y^4,$$

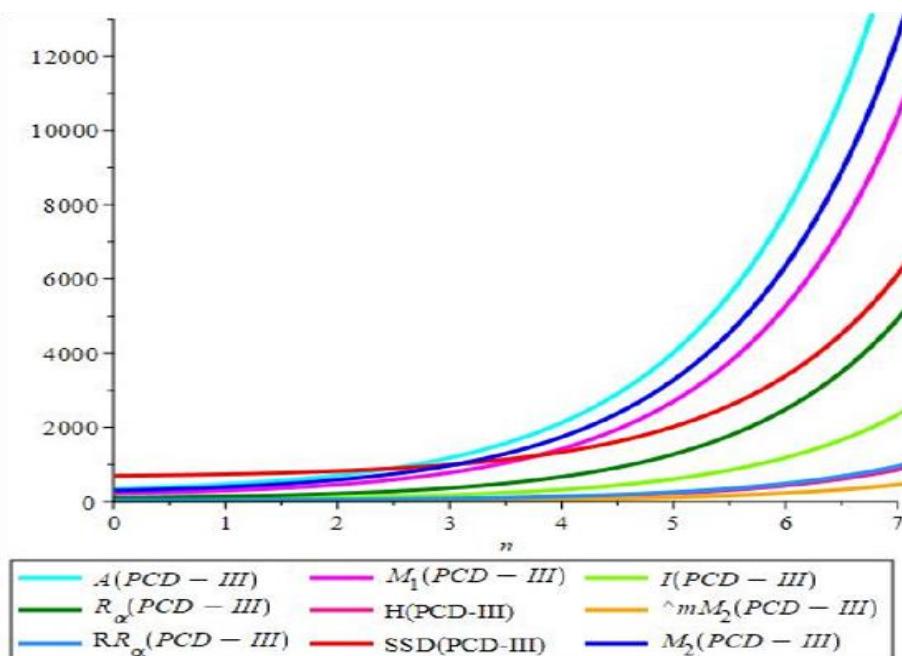
$$S_x J D_x D_y(f(x, y)) = (6 \times 2^n)x^4 + \frac{48}{5}x^5 + \frac{3}{2}(2^{n+3} + 12)x^6 + \frac{48}{7}x^7,$$

$$D_x^\alpha D_y^\alpha(f(x, y)) = (3^\alpha)(2^{n+3})xy^3 + 8(6^\alpha)x^2y^3 + 9^\alpha(2^{n+3} + 12)x^3y^3 + \frac{1}{9}(12^\alpha)x^3y^4,$$

$$S_x^\alpha S_y^\alpha(f(x, y)) = (\frac{1}{3})^\alpha(2^{n+3})xy^3 + 8(\frac{1}{6})^\alpha x^2y^3 + \frac{(2^{n+3} + 12)}{9^\alpha}x^3y^3 + 4(\frac{1}{12^\alpha})x^3y^4,$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) = (27 \times 2^n)x^2 + 64x^3 + \frac{729}{16}(2^{n+1} + 3)x^4 + \frac{192}{125}x^5.$$

Now, using [Table 1](#), the proof is complete.



**Figure 10:** Plot of comparison topological indices of *PCD-II*

#### *Porphyrin-cored dendrimer-IV (PCD-IV)*

The molecular diagram *PCD-IV* of generation  $G_n$  with  $n \geq 1$ . The (*PCD-IV*) is composed of twelve similar branches, such that one core is at its center. The central core is composed of 25 vertex, and 44 edges, as indicated in [Figure 11](#). According to [Table 8](#) and using degree-sum formula, the total number of edges in *PCD-IV* is  $24 \times 2^n + 20$  [3].

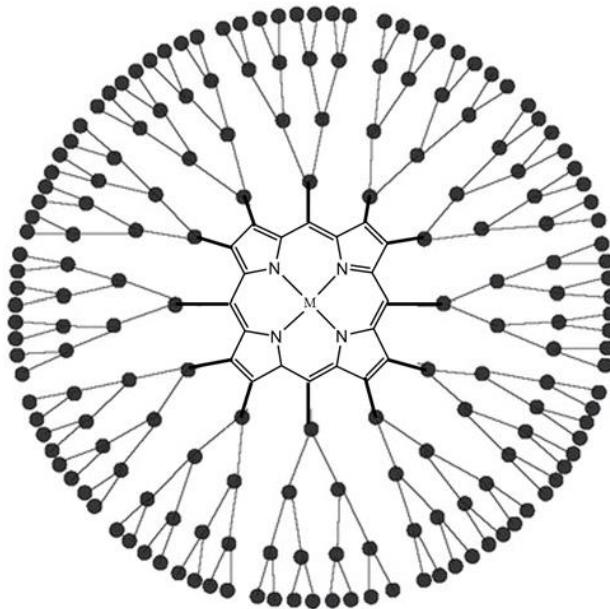
In [Figure 11](#), according to degrees of the vertex incident with each edge, set of edges *PCD-IV* can

be partitioned into 3 categories. We compute their cardinalities in [Table 9](#).

$$E(1,3) = \{uv \in E(\text{PCD-IV}) \mid d_u = 1, d_v = 3\},$$

$$E(3,3) = \{uv \in E(\text{PCD-IV}) \mid d_u = 3, d_v = 3\},$$

$$E(3,4) = \{uv \in E(\text{PCD-IV}) \mid d_u = 3, d_v = 4\}.$$

**Figure 11:** The molecular diagram of Porphyrin-cored dendrimer PCD-IV**Table 8:** The vertices partitions of PCD-IV

Degree of the vertex	Central core	In one of the branches	Total number of vertices
1	-	$2^n$	$2^{n+3}$
2	4	-	4
3	20	$2^n - 1$	$2^{n+3} + 12$
4	1	-	1
Total number of vertices	25	$2^{n+1} - 1$	$2^{n+4} + 17$

**Table 9:** The edges partitions of PCD - IV

$E(i, j)$	Number of edges
$E(1, 3)$	$12 \times 2^n$
$E(3, 3)$	$12 \times 2^n + 16$
$E(3, 4)$	4

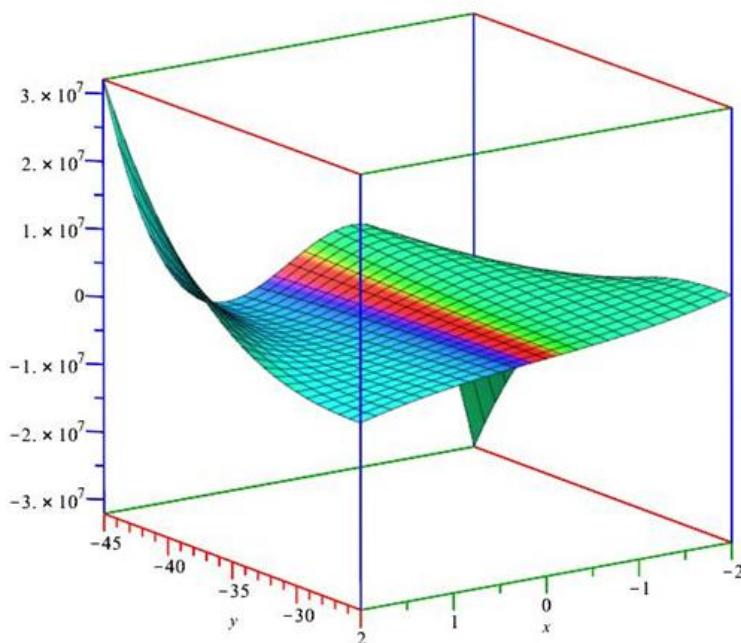
**Theorem 7.** Suppose  $M(PCD-IV; x, y)$  be M-Polynomial of PCD-IV. Then, we have:

$$M(PCD-IV; x, y) = (12 \times 2^n)xy^3 + (12 \times 2^n + 16)x^3y^3 + 4x^3y^4.$$

**Proof.** From the edges partition of  $PCD - IV$  given in [Table 5](#) and using Definition 3, we have:

$$M(PCD-IV; x, y) = \sum_{i \leq j} m_{ij} x^i y^j$$

$$\begin{aligned}
 &= \sum_{uv \in E(1,3)} m_{13}x^1y^3 + \sum_{uv \in E(3,3)} m_{33}x^3y^3 + \sum_{uv \in E(3,4)} m_{34}x^3y^4 \\
 &= |E(1,3)|x^1y^3 + |E(3,3)|x^3y^3 + |E(3,4)|x^3y^4 \\
 &= (12 \times 2^n)xy^3 + (12 \times 2^n + 16)x^3y^3 + 4x^3y^4.
 \end{aligned}$$



**Figure 12:** Plot of M-polynomial PCD-IV of generation  $G_3$

**Proposition 8.** Let PCD-IV be a molecule graph of generation  $G_n$  with  $n \geq 1$  growth stage, then

$$(1) \quad M_1(PCD-IV) = 120(2^n) + 124,$$

$$(2) \quad M_2(PCD-IV) = 144(2^n) + 192,$$

$$(3) \quad {}^mM_2(PCD-IV) = \frac{16}{3}(2^n) + \frac{19}{9},$$

$$(4) \quad R_\alpha(PCD-IV) = 3^\alpha(12 \times 2^n) + 9^\alpha(12 \times 2^n + 16) + 12^\alpha(4),$$

$$(5) \quad RR_\alpha(PCD-IV) = \frac{1}{3^\alpha}(12 \times 2^n) + \frac{1}{9^\alpha}(12 \times 2^n + 16) + \frac{1}{12^\alpha}(4),$$

$$(6) \quad SSD(PCD-IV) = 64(2^n) + \frac{121}{3},$$

$$(7) \quad H(PCD-IV) = 10(2^n) + \frac{136}{21},$$

$$(8) \quad I(PCD-IV) = 27(2^n) + \frac{216}{7},$$

$$(9) \quad A( PCD - IV ) = \frac{2835}{16} (2^n) + \frac{118773}{500}.$$

**Proof.** Let  $f(x, y) = (3 \times 2^{n+2})xy^3 + (3 \times 2^{n+2} + 16)x^3y^3 + 4x^3y^4$ ,

Then,

$$D_x(f(x, y)) = (3 \times 2^{n+2})xy^3 + 3(3 \times 2^{n+2} + 16)x^3y^3 + 12x^3y^4,$$

$$D_y(f(x, y)) = (9 \times 2^{n+2})xy^3 + 3(3 \times 2^{n+2} + 16)x^3y^3 + 16x^3y^4,$$

$$D_x D_y(f(x, y)) = 3(12 \times 2^n)xy^3 + 9(12 \times 2^n + 16)x^3y^3 + 48x^3y^4,$$

$$S_x(f(x, y)) = (3 \times 2^{n+2})xy^3 + \frac{1}{3}(3 \times 2^{n+2} + 16)x^3y^3 + \frac{4}{3}x^3y^4,$$

$$S_y(f(x, y)) = 2^{n+2}xy^3 + \frac{1}{3}(3 \times 2^{n+2} + 16)x^3y^3 + x^3y^4,$$

$$S_x S_y(f(x, y)) = 2^{n+2}xy^3 + \frac{1}{9}(3 \times 2^{n+2} + 16)x^3y^3 + \frac{1}{3}x^3y^4,$$

$$D_x S_y(f(x, y)) = 2^{n+2}xy^3 + (3 \times 2^{n+2} + 16)x^3y^3 + 3x^3y^4,$$

$$S_x D_y(f(x, y)) = (9 \times 2^{n+2})xy^3 + (3 \times 2^{n+2} + 16)x^3y^3 + \frac{16}{3}x^3y^4,$$

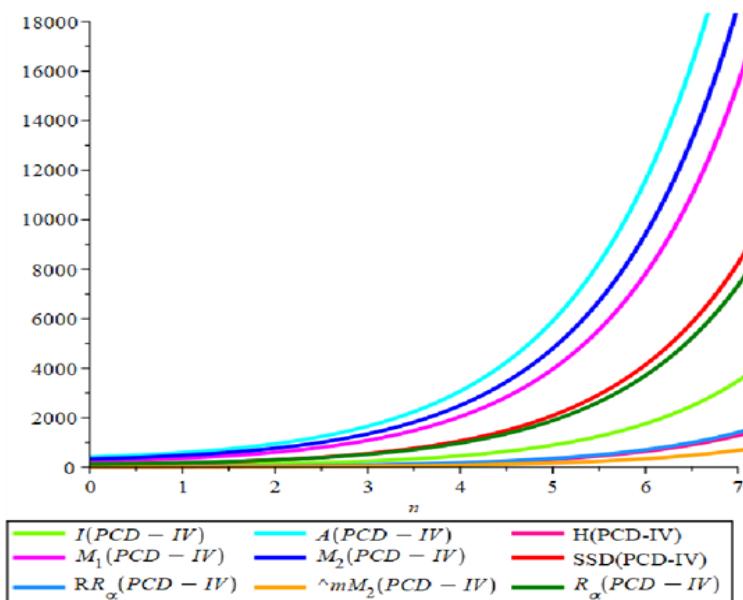
$$S_x J D_x D_y(f(x, y)) = (3 \times 2^n)x^4 + \frac{1}{6}(3 \times 2^{n+2} + 16)x^6 + \frac{4}{7}x^7,$$

$$D_x^\alpha D_y^\alpha(f(x, y)) = (3^{\alpha+1})(2^{n+2})xy^3 + 9^\alpha(3 \times 2^{n+2} + 16)x^3y^3 + 4(12^\alpha)x^3y^4,$$

$$S_x^\alpha S_y^\alpha(f(x, y)) = (\frac{1}{3})^\alpha(3 \times 2^{n+2})xy^3 + \frac{(3 \times 2^{n+2} + 16)}{9^\alpha}x^3y^3 + 4(\frac{1}{12^\alpha})x^3y^4,$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) = (81 \times 2^{n-1})x^2 + \frac{729}{64}(3 \times 2^{n+2} + 16)x^4 + \frac{6912}{125}x^5.$$

Now, using [Table 1](#), the proof is complete.

**Figure 13:** Plot of comparison topological indices of PCD-IV

## Conclusion

According to Figures 4, 7, 10, and, 13, all diagrams are exponential functions with base 2, and they are increasing with the increase in the number of generations. In dendrimers *PCD-I*, *PCD-II*, and *PCD-IV*, the Augmented Zagreb index value is the highest, and the Second Modified Zagreb index value is the lowest, while in *PCD-III*, up to the 3<sup>rd</sup> generation, the Symmetric Division Index value is the highest. In all four types of porphyrin-cored dendrimers, the numerical values of the General Randić and the Harmonic indices almost are very close to each other. In *PCD-I*, in the higher generations, the First Zagreb and the Second Zagreb indices, and also the Inverse Randić and Symmetric Division indices, coincide. Figures 3, 6, 9, and, 12 show that amounts computed using M-Polynomial have various behaviors related to parameters of x and y. The results obtained in this article will help researchers to observe the strong correlation between the physicochemical properties of dendrimers and topological indices in the study of drugs.

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## Authors' contributions

All authors contributed to data analysis, drafting, and revising of the paper and agreed to be responsible for all the aspects of this work.

## Conflict of Interest

We have no conflicts of interest to disclose.

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