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Gourava Indices of Some Dendrimer Structures

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ABSTRACT

In Chemical Science, the topological indices are used in the analysis of drug molecular structures. These indices are helpful for chemical scientists to find out the chemical and biological characteristics of drugs. In this study, we compute and obtain the comparative analysis of the Gourava indices and hyper Gourava indices of some important class of dendrimers which appeared in nanosciences.

1. Introduction

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(v)$ of a vertex v is the number of vertices adjacent to v. For all further notations and terminology, we refer to [1].

A molecular graph or chemical graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. In nanoscience, concerning the definition of the topological index on the molecular graph and corresponding chemical, pharmaceutical properties of drugs can be studied by the topological index calculation, see [2, 3].

The first and second Gourava indices [4] of a graph G are defined as

$$GO_1(G) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v)+d_G(u)d_G(v)]\cdots\cdots(1)$$

$$GO_2(G) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v))(d_G(u)d_G(v))]\cdots\cdots(2)$$

In [5], Kulli introduced the first and second hyper Gourava indices of a graph, defined as

$$HGO_1(G) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v))+d_G(u)d_G(v)]^2\cdots\cdots(3)$$

$$HGO_2(G) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v))(d_G(u)d_G(v))]^2\cdots\cdots(4)$$

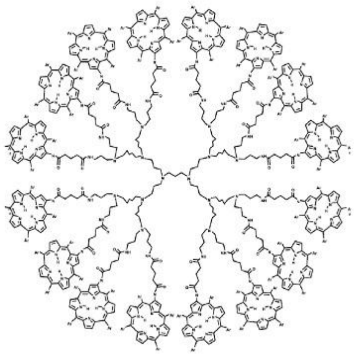
Recently, some novel variants of Gourava indices were introduced and studied such as the product connectivity Gourava index [6], sum connectivity Gourava index [7].

In this paper, we compute the Gourava indices and hyper Gourava indices of porphyrin dendrimer, prophl ether imine dendrimer, zinc porphyrin dendrimer and poly ethylene amide amine dendrimer. Some degree based topological indices eccentricity based topological indices of these dendrimers were studied in [8, 9, 10, 11].

2. Porphyrin Dendrimer

The family of porphyrin dendrimers is denoted by D_nP_n where n is the steps of growth in this type of dendrimers. The graph of D_nP_n is presented in Figure 1.

Figure -1: The graph of D_nP_n



Let $G = D_nP_n$. By algebraic method, we obtain that D_nP_n has $96n – 10$ vertices and $105n – 11$ edges. In Porphyrin dendrimer D_nP_n, these are six different types of edges based on degree of end vertices of each edge. Also by algebraic method, we obtain six edge partitions of D_nP_n as given in Table 1.

Table-1: Edge partition of D_nP_n

$d_G(u)$, $d_G(v)$: uv $E(G)$	(1,2)	(1, 4)	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	2n	24n	10n- 5	48n- 6	13n	8n

Theorem 1. Let D_nP_n be a porphyrin dendrimer. The first and the second Gourava indices of D_nP_n are

(a) $GO_1(D_nP_n) = 1185n – 106$.
(b) $GO_2(D_nP_n) = 3478n – 260$

Proof **:** Let $G = D_nP_n$. (a) By definition, we have

$$GO_1(DnPn) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v)+d_G(u)d_G(v)]$$

Then using the information given in Table-1, we have

$GO_1(D_nP_n) = [(1 + 3) + (1 \times 3)]2n + [(1 + 4) + (1 \times 4)]24n$
$+ [(2 + 2) + (2 \times 2)](10n - 5) - [(2 + 3)$
$+ (2 \times 3)](48n - 6) + [(3 + 3) + (3 \times 3)]13n$
$+ [(3 + 4) + (3 \times 4)]8n.$
$= 1185n - 106.$

(b) By definition, we have

$$GO_2(DnPn) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u) d_G(v))]$$

Then using the information given in Table-1, we obtain

$GO_2(D_nP_n) = [(1 + 3) \times (1 \times 3)]2n + [(1 + 4) \times (1 \times 4)]24n$
$+ [(2 + 2) \times (2 \times 2)](10n - 5) + [(2 + 3)$
$\times (2 \times 3)](48n - 6) + [(3 +3) \times (3 \times 3)]13n$
$+ [(3 + 4) \times (3 \times 4)]8n$
$= 3478n - 260$

Theorem 2. The first and second hyper Gourava indices of D_nP_n are

(a) $HGO_1(D_nP_n) = 14303n - 1046$
(b) $HGO_2(D_nP_n) = 150004n - 6680.$

Proof **:** Let $G = D_nP_n$. (a) By definition, we have

$$HGO_1(DnPn) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + d_G(u) d_G(v)]^2$$

Then using the information given in Table-1, we deduce

$HGO_1(D_nP_n) = [(1 + 3) + (1 \times 3)]^2 2n + [(1 +4) + (1 \times 4)]^2\ 24n$
$+ [(2 + 2)+(2 \times 2)]^2(10n - 5) + [(2 + 3)$
$+ (2 \times 3)]^2(48n - 6) + [(3 + 3) + (3 \times 3)]^2 13n$
$+ [(3 + 4) + (3 \times 4)]^2 8n.$
$= 14303n - 1046.$

(b) By definition, we have

$$HGO_2(DnPn) \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u) d_G(v))]^2$$

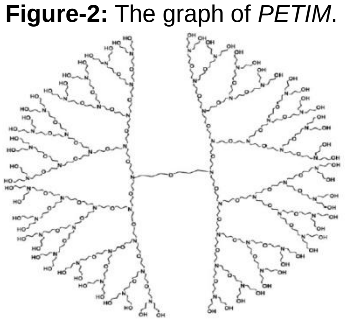
Thus by using Table 1, we derive

$HGO_2(D_nP_n) = [(1 + 3)(1 \times 3)]^2 2n + [(1 + 4)(1 \times 4)]^2 24n$
$+ [(2 + 2)(2 \times 2)]^2(10n - 5) + [(2 + 3)(2 \times 3)]^2$
$(48n - 6) + [(3 + 3)(3 \times 3)]^2 13n$
$+ [(3 + 4)(3 \times 4)]^2 8n.$
$= 150004n - 6680.$

3. Results for Propyl ether Imine Dendrimer

We consider the family of Propyl ether imine dendrimers and it is denoted by *PETIM*. The graph of *PETIM* is presented in Figure-2.

Figure-2: The graph of *PETIM*.



Let *G* be the graph of *PETIM* dendrimer. By calculation, we have $|V(G)| = 24 \times 2^n - 23$ and $|E(G)| = 24 \times 2^n - 24$. In *G*, there are three types of edges based on the degree of end vertices of each edge as given in Table-2.

Table-2: Edge partition of *PETIM*

$d_G(u), d_G(v) : uv \in E(G)$	(1, 2)	(2, 2)	(2, 3)
Number of edges	2×2^n	$16 \times 2^n - 18$	$6 \times 2^n - 6$

Theorem 3. Let *G* be the graph of *PETIM* dendrimer. The first and second Gourava indices of *PETIM* are

(a) $GO_1(PETIM) = 204 \times 2^n - 210.$
(b) $GO_2(PETIM) = 448 \times 2^n - 468.$

Proof : (a) By using equation (1) and Table-3, we deduce

$$GO_1(PETIM) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v) + d_G(u) d_G(v)]$$

$= [(1 + 2) + (1 \times 2)]\ 2 \times 2^n + [(2 + 2)$
$+ (2 \times 2)]\ (16 \times 2^n - 18) + [(2 + 3)$
$+ (2 \times 3)](\ 6 \times 2^n - 6).$
$= 204 \times 2^n - 210.$

(b) From equation (2) and by using Table 2, we derive

$$GO_2(PETIM) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u) d_G(v))]$$

$= [(1 + 2)(1 \times 2)]\ 2 \times 2^n + [(2 + 2)(2 \times 2)]$
$(16 \times 2^n - 18) + [(2 + 3)(2 \times 3)](\ 6 \times 2^n - 6).$
$= 448 \times 2^n - 468.$

Theorem 4. Let *G* be the graph of *PETIM* dendrimer. The first and second hyper Gourava indices of *PETIM* are

(a) $HGO_1(PETIM) = 1800 \times 2^n - 1014$
(b) $HGO_2(PETIM) = 9568 \times 2^n - 10008$

Proof : (a) from equation (3) and by using Table 2, we obtain

$$HGO_1(PETIM) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v)) + d_G(u) d_G(v)]^2$$

$= [(1 + 2) + (1 \times 2)]^2\ 2 \times 2^n + [(2 + 2)$
$+ (2 \times 2)]^2\ (16 \times 2^n - 18) + [(2 + 3)$
$+ (2 \times 3)]^2\ (\ 6 \times 2^n - 6).$
$= 1800 \times 2^n - 1014.$

(b) By using equation (4) and Table 2. We have

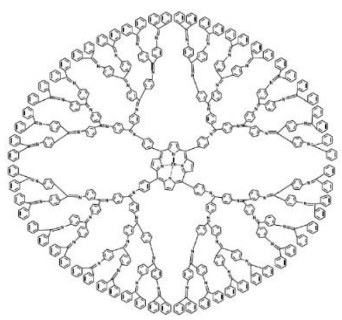
$$HGO_2(PETIM) = \sum_{uv \in E(G)} [(d_G(u) + d_G(v))(d_G(u) d_G(v))]^2$$

$= [(1 + 2)(1 \times 2)]^2\ 2 \times 2^n + [(2 + 2)(2 \times 2)]^2$
$(16 \times 2^n - 18) + [(2 + 3)(2 \times 3)]^2$
$(6 \times 2^n - 6).$
$= 9568 \times 2^n - 10008.$

4. Results for Zinc Porphyrin dendrimer

We consider the family of zinc porphyrin dendrimers which is denoted by *DPZn*. The graph of *DPZn* is shown in Figure-3.

Figure-3: The graph of *DPZn*.



Let *G* be the graph of *DPZn* dendrimer. By calculation, we have $|V(G)| = 56 \times 2^n - 7$ and $|E(G)| = 64 \times 2^n - 4$. In *G*, there are four types of edges based on the degree of end vertices of each edge as given in Table-3.

Table-3: Edge partition graph of DPZ_n.

$d_G(u),d_G(v)$: $uv \in E(G)$	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$16 \times 2^n - 4$	$40 \times 2^n - 6$	$8 \times 2^n + 12$	4

***Theorem* 5.** Let G be the graph of *DPZn* dendrimer. The first and second Gourava indices of *DPZn* are

(a) $GO_1(DPZn) = 688 \times 2^n + 98$

(b) $GO_2(DPZn) = 808 \times 2^n + 740$

Proof : (a) By using equation (1) and Table 3, we derive

$$GO_1(DPZn) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v)+d_G(u)d_G(v)]$$

$$= [(2+2) + (2 \times 2)](16 \times 2^n - 4) + [(2 + 3) + (2 \times 3)](40 \times 2^n - 6) + [(3 + 3) + (3 \times 3)](8 \times 2^n + 12) + [(3 + 4) + (3 \times 4)]4$$

$$= 688 \times 2^n + 98.$$

(b) From equation (2) and by using Table 3, we deduce

$$GO_2(DPZn) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v))(d_G(u)d_G(v))]$$

$$= [(2+2)(2 \times 2)](16 \times 2^n - 4) + [(2 + 3)(2 \times 3)](40 \times 2^n - 6) + [(3 + 3)(3 \times 3)](8 \times 2^n + 12) + [(3 + 4)(3 \times 4)]4$$

$$= 808 \times 2^n + 740.$$

***Theorem* 6**. Let G be the graph of *DPZn* dendrimer. The first and second hyper Gourava indices of *DPZn* are

(a) $HGO_1(DPZn) = 7664 \times 2^n + 3162$

(b) $HGO_2(DPZn) = 63424 \times 2^n + 56792$

***Proof* :** (a) By using equation (3) and Table 3, we obtain

$$HGO_1(DPZn) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v))+d_G(u)d_G(v)]^2$$

$$= [(2 + 2) + (2 \times 2)]^2 (16 \times 2^n - 4) + [(2 + 3) + (2 \times 3)]^2(40 \times 2^n - 6) + [(3 + 3) + (3 \times 3)]^2 (8 \times 2^n + 12) + [(3 + 4) + (3 \times 4)]^2 4.$$

$$= 7664 \times 2^n + 3162$$

(b) From equation (2) and by using Table 3, we deduce

$$HGO_2(DPZn) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v))(d_G(u)d_G(v))]^2$$

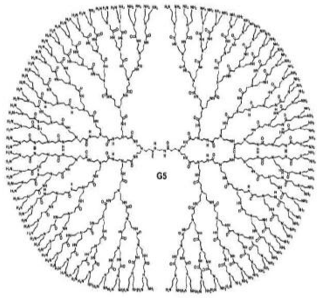
$$= [(2 + 2)(2 \times 2)]^2 (16 \times 2^n - 4) + [(2 + 3)(2 \times 3)]^2 (40 \times 2^n - 6) + [(3 + 3)(3 \times 3)]^2 (8 \times 2^n + 12) + [(3 + 4)(3 \times 4)]^2 4.$$

$$= 63424 \times 2^n + 56792.$$

1. Results for Poly Ethylene Amide Amine Dendrimer

We consider the family of poly ethylene amide amine dendrimers which is denoted by *PETAA*. The graph of *PETAA* is depicted in Figure 4.

Figure-4: The graph of *PETAA*



Let G be the graph of *PETAA* dendrimer. By calculation, we have $|V(G)| = 44 \times 2^n - 18$ and $|E(G)| = 44 \times 2^n - 19$. In G, there are four types of edge based on degree of end vertices of each edge as given in Table-4.

Table-4: Edge partition of *PETAA*

$d_G(u),d_G(v)$: $uv \in E(G)$	(1, 2)	(1, 3)	(2, 2)	(2, 3)
Number of edges	4×2^n	$4 \times 2^n - 2$	$16 \times 2^n - 8$	$20 \times 2^n - 9$

***Theorem* 7.** Let G be the graph of *PETAA* dendrimer. The first and second Gourava indices of *PETAA* are

(a) $GO_1(PETAA) = 396 \times 2^n - 177$

(b) $GO_2(PETAA) = 928 \times 2^n - 422$

Proof : (a) By using equation (1) and Table 4, we obtain

$$GO_1(PETAA) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v)+d_G(u)d_G(v)]$$

$$= [(1 + 2) + (1 \times 2)]\, 4 \times 2^n + [(1 + 3) + (1 \times 3)](4 \times 2^n - 2) + [(2 + 2) + (2 \times 2)](16 \times 2^n - 8) + [(2 + 3) + (2 \times 3)]\,(20 \times 2^n - 9)$$

$$= 396 \times 2^n - 177.$$

(b) From equation (2) and by using Table 4, we deduce

$$GO_2(PETAA) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v))(d_G(u)d_G(v))]$$

$$= [(1 + 2)(1 \times 2)]\, 4 \times 2^n + [(1 + 3)(1 \times 3)](4 \times 2^n - 2) + [(2 + 2)(2 \times 2)]\,(16 \times 2^n - 8) + [(2 + 3)(2 \times 3)]\,(20 \times 2^n - 9)$$

$$= 928 \times 2^n - 422.$$

***Theorem* 8.** Let G be the graph of *PETAA* dendrimer. The first and second hyper Gourava indices of *PETAA* are

(a) $HGO_1(PETAA) = 3740 \times 2^n - 1699$

(b) $HGO_2(PETAA) = 22816 \times 2^n - 10436.$

Proof : (a) By using equation (3) and Table 4, we obtain

$$HGO_1(PETAA) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v))+d_G(u)d_G(v)]^2$$

$$= [(1 + 2) + (1 \times 2)]^2\, 4 \times 2^n + [(1 + 3) + (1 \times 3)]^2 (4 \times 2^n - 2) + [(2 + 2) + (2 \times 2)]^2 (16 \times 2^n - 8) + [(2 + 3) + (2 \times 3)]^2 (20 \times 2^n - 9)$$

$$= 3740 \times 2^n - 1699.$$

(b) From equation (4) and by using Table 4, we deduce

$$HGO_2(PETAA) = \sum_{uv\in E(G)}[(d_G(u)+d_G(v))(d_G(u)d_G(v))]^2$$

$$= [(1 + 2)(1 \times 2)]^2\, 4 \times 2^n + [(1 + 3)(1 \times 3)]^2 (4 \times 2^n - 2) + [(2 + 2)(2 \times 2)]^2 (16 \times 2^n - 8) + [(2 + 3)(2 \times 3)]^2 (20 \times 2^n - 9)$$

$$= 22816 \times 2^n - 10436.$$

2. Comparative Analysis and Conclusion

Figure -5: Plot of Gourava indices(GO_1) for dendrimers

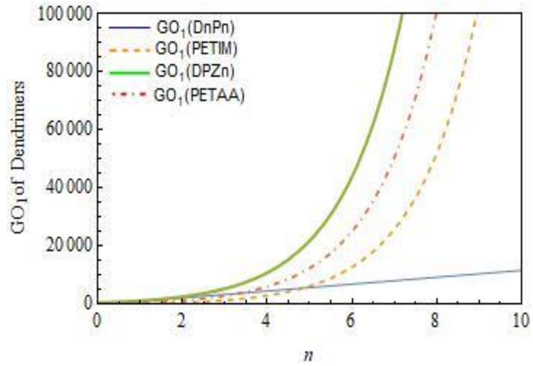


Figure-6: Plot of Gourava indices(GO_2) for dendrimers

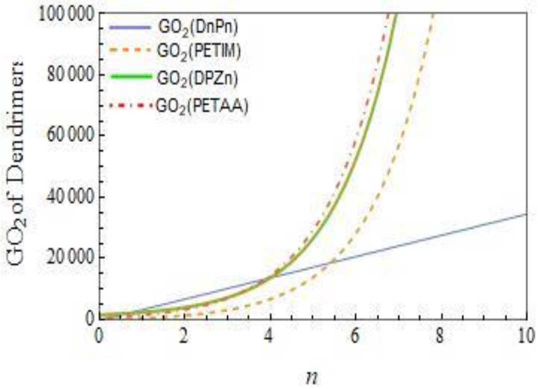


Figure -7 : Plot of hyper Gourava indices(HGO_1) for dendrimers

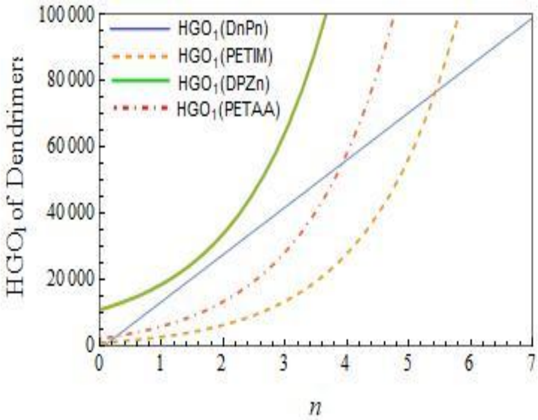
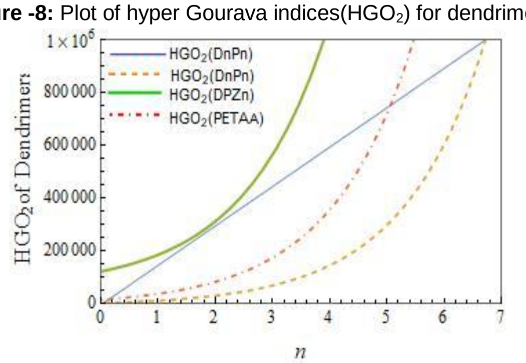


Figure -8: Plot of hyper Gourava indices(HGO_2) for dendrimers



Figures-5, 6, 7 and 8 shows that $GO_1(DnPn)$, $GO_2(DnPn)$, $HGO_1(DnPn)$, $HGO_2(DnPn)$ are linearly increasing and $GO_1(PETIM)$, $GO_2(PETIM)$, $HGO_1(PETIM)$, $HGO_2(PETIM)$, $GO_1(DPZn)$, $GO_2(DPZn)$, $HGO_1(DPZn)$, $HGO_2(DPZn)$, $GO_1(PETAA)$, $GO_2(PETAA)$, $HGO_1(PETAA)$, $HGO_2(PETAA)$ are exponentially increasing, if we further increase the value of *n*, then these exponentially increasing curves attains saturation. Figure-6 shows that the saturation points are very close for $GO_2(DPZn)$ and $GO_2(PETAA)$. The co-efficient of correlation R^2 for $GO_1(DnPn)$, $GO_2(DnPn)$, $HGO_1(DnPn)$, $HGO_2(DnPn)$ is 1 which shows that the line is linearly fitted. This shows that the Gourava and hyper Gourava indices are theoretically fit for dendrimer *DnPn*.

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