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GOURAVA SOMBOR INDICES

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ABSTRACT

In this paper, we introduce the Gourava Sombor index, the reduced Gourava Sombor index and their corresponding exponentials of a graph. Also we compute these newly defined Gourava Sombor indices and their corresponding exponentials for some important nanostructures which are appeared in nanoscience.

Keywords: Gourava Sombor index, reduced Gouravs Sombor index, nanostructures.

Mathematics Subject Classification : 05C05, 05C12, 05C35.

1. INTRODUCTION

The simple, connected graph *G* is with vertex set *V*(*G*) and edge set *E*(*G*). The number of vertices adjacent to the vertex *u* called degree of *u*, denoted by *d*(*u*). The edge *e* incident by the vertices *u* and *v* with edge *uv*=*e*. Define *d*(*e*) = *d*(*u*) + *d*(*v*) – 2. For other graph terminologies and notions, the readers are referred to books [1, 2, 3].

A chemical graph is a graph whose vertices correspond to the atom and edges to the bonds. Mathematical Chemistry is very useful in the study of Chemical Sciences. We have found many applications in Mathematical Chemistry by using graph indices, especially in QSPR/QSAR research [4].

Kulli [5] introduced the first and second Gourava indices of a graph *G* are

$$GO_1(G)=\sum_{uv\in E(G)}\left[d(u)+d(v)+d(u)d(v)\right],$$

$$GO_2(G)=\sum_{uv\in E(G)}\left(d(u)+d(v)\right)d(u)d(v).$$

Recently, some Gourava indices were studied, for example, in [6, 7, 8, 9, 10].

Gutman [11] introduced the Sombor index of a graph *G* is

$$SO(G)=\sum_{uv\in E(G)}\sqrt{d(u)^2+d(v)^2}.$$

Recently, some Sombor indices were studied, for example, in [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27].

Motivated by the definition of the Sombor index and its wide applications, we propose Gourava Sombor index of a graph as follows:

The Gourava Sombor index of a graph *G* is defined as

$$GSO(G)=\sum_{uv\in E(G)}\left[\left(d(u)+d(v)\right)^2+\left(d(u)d(v)\right)^2\right]^{\frac{1}{2}}.$$

In view of the Gourava Sombor index, we propose the Gourava Sombor exponential of a graph *G* and it is defined as

$$GSO(G,x)=\sum_{uv\in E(G)}x^{\left[\left(d(u)+d(v)\right)^2+\left(d(u)d(v)\right)^2\right]^{\frac{1}{2}}}.$$

We propose the reduced Gourava Sombor index of a graph *G* and it is defined as

$$RGSO(G)=\sum_{uv\in E(G)}\left[\left(d(u)-1+d(v)-1\right)^2+\left((d(u)-1)(d(v)-1)\right)^2\right]^{\frac{1}{2}}.$$

In view of the reduced Gourava Sombor index, we introduce the reduced Gourava Sombor exponential of a graph *G* and it is defined as

$$RGSO(G,x)=\sum_{uv\in E(G)}x^{\left[\left(d(u)-1+d(v)-1\right)^2+\left((d(u)-1)(d(v)-1)\right)^2\right]^{\frac{1}{2}}}.$$

In this paper, the Gourava Sombor and reduced Gourava Sombor indices for certain nanostructures are determined.

2. SOME STANDARD GRAPHS

Theorem 1. If $K_{m,n}$ is a complete bipartite graph with $1 \le m \le n$, then

$$GSO(K_{m,n})=mn\sqrt{(m+n)^2+(mn)^2}.$$

Proof: Let $K_{m,n}$ be a complete bipartite graph with $m + n$ vertices and mn edges such that $|V_1| = m$, $|V_2| = n$, $V(K_{m,n}) = V_1 \cup V_2$. Every vertex of V_1 is adjacent with *n* vertices and every vertex of V_2 is adjacent with *m* vertices.

$$GSO(K_{m,n})=mn\sqrt{(m+n)^2+(mn)^2}.$$

Corollary 1.1. Let $K_{n,n}$ be a complete bipartite graph with $n \ge 2$ vertices. Then

$$GSO(K_{n,n})=n^3\sqrt{4+n^2}.$$

Corollary 1.2. Let $K_{1,n}$ be a star with $n\ge2$ vertices. Then

$$GSO(K_{1,n})=n\sqrt{(1+n)^2+n^2}.$$

Theorem 2. If *G* is an *r*-regular graph with $n \ge 2$ vertices, then

$$GSO(G)=\frac{nr^2}{2}\sqrt{4+r^2}.$$

Proof: Let *G* be an r-regular graph with *n* vertices and $\frac{nr}{2}$ edges. Then the degree of each vertex of *G* is *r*.

$$GSO(G)=\frac{nr}{2}\sqrt{(r+r)^2+(r^2)^2}=\frac{nr^2}{2}\sqrt{4+r^2}.$$

Corollary 1. If C_n is a cycle with $n\ge3$ vertices, then

$$GSO(C_n)=4\sqrt{2}n.$$

Corollary 2. If K_n is a complete graph with $n\ge2$ vertices, then

$$GSO(K_n)=\frac{1}{2}n(n-1)^2\sqrt{(n^2-2n+5)}.$$

Theorem 3. Let P_n be a path with $n\geq3$ vertices. Then G_4

$$GSO(P_n)=4\sqrt{2}n+2\sqrt{13}-12\sqrt{2}.$$

Proof: Let P_n be a path with $n\geq3$ vertices. We obtain two partitions of the edge set of P_n as follows:

$E_3 = \{uv \in E(P_n) \mid d_G(u)=1, d_G(v)=2\}, |E_3| = 2.$

$E_4 = \{uv \in E(P_n) \mid d_G(u) = d_G(v)=2\}, |E_4| = n-3.$

To compute $NGO(P_n)$, we see that

$$GSO(P_n)=\sqrt{(1+2)^2+(1\times2)^2}\,2+\sqrt{(2+2)^2+(2\times2)^2}\,(n-3)$$
$$=4\sqrt{2}n+2\sqrt{13}-12\sqrt{2}.$$

3. POLY ETHYLENE AMIDE AMINE DENDRIMER *PETAA*

The chemical graphs G_1 of poly ethylene amide amine dendrimers *PETAA* structure have $44\times2^n-18$ vertices and $44\times2^n-19$ edges are shown in Figure 1.

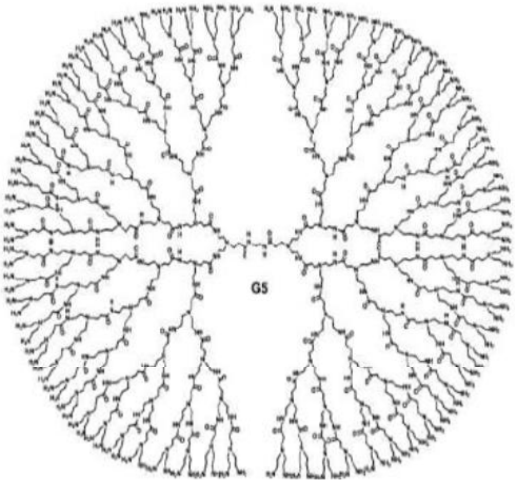

Figure 1. The molecular graph of *PETAA*

In the above structure, we obtain that $\{d(u),d(v): uv \in E(G_1)\}$ has four edge set partitions.

$d(u), d(v) \setminus uv \in E(G_1)$	(1, 2)	(1, 3)	(2, 2)	(2, 3)
Number of edges	4×2^n	$4\times2^n-2$	$16\times2^n-8$	$20\times2^n-9$

Table 1. Edge set partition of *PETAA*

We calculate the Gourava Sombor index of *PETAA* chemical graph as follows:

Theorem 1. Let G_1 be the chemical structure of *PETAA*. Then

$$GSO(G_1)=\left(4\sqrt{13}+20+64\sqrt{2}+20\sqrt{61}\right)2^n-10-32\sqrt{2}-9\sqrt{61}.$$

Proof: Applying definition and edge set partition of G, we conclude

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$$GSO(G_1)=\sum_{uv\in E(G_1)}\left[\left(d(u)+d(v)\right)^2+\left(d(u)d(v)\right)^2\right]^{\frac{1}{2}}.$$

$$=4\times 2^n\left[(1+2)^2+(1\times 2)^2\right]^{\frac{1}{2}}+\left(4\times 2^n-2\right)\left[(1+3)^2+(1\times 3)^2\right]^{\frac{1}{2}}$$

$$+\left(16\times 2^n-8\right)\left[(2+2)^2+(2\times 2)^2\right]^{\frac{1}{2}}+\left(20\times 2^n-9\right)\left[(2+3)^2+(2\times 3)^2\right]^{\frac{1}{2}}.$$

By simplifying the above equation, we obtain the necessary result.

We calculate the reduced Gourava Sombor index of *PETAA* chemical graph as follows:

Theorem 2. Let G_1 be the chemical structure of *PETAA*. Then

$$RGSO(G_1)=\left(12+16\sqrt{5}+20\sqrt{13}\right)2^n-4-8\sqrt{5}-9\sqrt{13}.$$

Proof: Applying definition and edge set partition of G_1, we conclude

$$RGSO(G_1)=\sum_{uv\in E(G_1)}\left[\left(d(u)-1+d(v)-1\right)^2+\left((d(u)-1)(d(v)-1)\right)^2\right]^{\frac{1}{2}}$$

$$=4\times 2^n\left[(0+1)^2+(0\times 1)^2\right]^{\frac{1}{2}}+\left(4\times 2^n-2\right)\left[(0+2)^2+(0\times 2)^2\right]^{\frac{1}{2}}$$

$$+\left(16\times 2^n-8\right)\left[(1+1)^2+(1\times 1)^2\right]^{\frac{1}{2}}+\left(20\times 2^n-9\right)\left[(1+2)^2+(1\times 2)^2\right]^{\frac{1}{2}}$$

By solving the above equation, we get the desired result.

By using definitions and Table 1, we obtain the Gourava Sombor and reduced Gourava Sombor exponentials of *PETAA* chemical graph as follows:

Theorem 3. The Gourava Sombor exponential of *PETAA* is given by

$$GSO(G_1,x)=\left(4\times 2^n\right)x^{\sqrt{13}}+\left(4\times 2^n-2\right)x^5+\left(16\times 2^n-8\right)x^{4\sqrt{2}}+\left(20\times 2^n-9\right)x^{\sqrt{61}}.$$

Theorem 4. The reduced Gourava Sombor index of *PETAA* is given by

$$RGSO(G_1,x)=\left(4\times 2^n\right)x^1+\left(4\times 2^n-2\right)x^2+\left(16\times 2^n-8\right)x^{\sqrt{5}}+\left(20\times 2^n-9\right)x^{\sqrt{13}}.$$

4. PROPYL ETHER IMINE DENDRIMER *PETIM*

The chemical graphs G_2 of propyl ether imine dendrimers *PETIM* structure have $24\times 2^n-23$ vertices and $24\times 2^n-24$ edges are shown in Figure 2.

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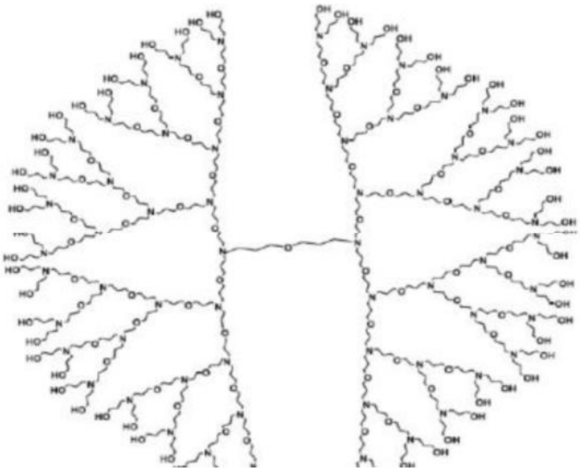

Figure 2. The molecular graph of *PETIM*

In the above structure, we obtain that $\{d(u),d(v): uv \in E(G_2)\}$ has three edge set partitions.

$d(u), d(v) \setminus uv \in E(G_2)$	(1, 2)	(2, 2)	(2, 3)
Number of edges	2×2^n	$16 \times 2^n - 18$	$6 \times 2^n - 6$

Table 2. Edge partition of *PETIM*

We calculate the Gourava Sombor index of *PETIM* chemical graph as follows:

Theorem 5. Let G_2 be the chemical structure of *PETIM*. Then

$$GSO(G_2) = \left(2\sqrt{13} + 64\sqrt{2} + 6\sqrt{61}\right)2^n - 72\sqrt{2} - 6\sqrt{61}.$$

Proof: Applying definition and edge set partition of G_2, we conclude

$$GSO(G_2) = \sum_{uv \in E(G_2)} \left[\left(d(u)+d(v)\right)^2 + \left(d(u)d(v)\right)^2\right]^{\frac{1}{2}}.$$

$$= 2 \times 2^n\left[(1+2)^2 + (1\times 2)^2\right]^{\frac{1}{2}} + \left(16 \times 2^n - 18\right)\left[(2+2)^2 + (2\times 2)^2\right]^{\frac{1}{2}}$$

$$+\left(6 \times 2^n - 6\right)\left[(2+3)^2 + (2\times 3)^2\right]^{\frac{1}{2}}.$$

By simplifying the above equation, we get the necessary result.

We calculate the reduced Gourava Sombor index of *PETIM* chemical graph as follows:

Theorem 6. Let G_2 be the chemical structure of *PETIM*. Then

$$RGSO(G_2) = \left(2 + 16\sqrt{5} + 6\sqrt{13}\right)2^n - 18\sqrt{5} - 6\sqrt{13}.$$

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Proof: Applying definition and edge set partition of G_2, we conclude

$$RGSO(G_2)=\sum_{uv\in E(G_2)}\left[\left(d(u)-1+d(v)-1\right)^2+\left((d(u)-1)(d(v)-1)\right)^2\right]^{\frac{1}{2}}.$$

$$=2\times 2^n\left[(0+1)^2+(0\times1)^2\right]^{\frac{1}{2}}+\left(16\times 2^n-18\right)\left[(1+1)^2+(1\times1)^2\right]^{\frac{1}{2}}$$

$$+\left(6\times 2^n-6\right)\left[(1+2)^2+(1\times2)^2\right]^{\frac{1}{2}}$$

By solving the above equation, we get the desired result.

By using definitions and Table 2, we estalish the Gourava Sombor and reduced Gourava Sombor exponentials of *PETIM* chemical graph as follows:

Theorem 7. The Gourava Sombor exponential of *PETIM* is given by

$$GSO(G_2,x)=\left(2\times2^n\right)x^{\sqrt{13}}+\left(16\times 2^n-18\right)x^{4\sqrt{2}}+\left(6\times 2^n-6\right)x^{\sqrt{61}}.$$

Theorem 8. The reduced Gourava Sombor exponential of *PETIM* is given by

$$RGSO(G_2,x)=\left(2\times2^n\right)x^{1}+\left(16\times 2^n-18\right)x^{\sqrt{5}}+\left(6\times 2^n-6\right)x^{\sqrt{13}}.$$

5. ZINC PROPHYRIN DENDRIMER DPZ_n

The chemical graphs G_3 of zinc prophyrin dendrimers DPZ_n structure have $56\times2^n-7$ vertices and $64\times2^n-4$ edges are shown in Figure 3.

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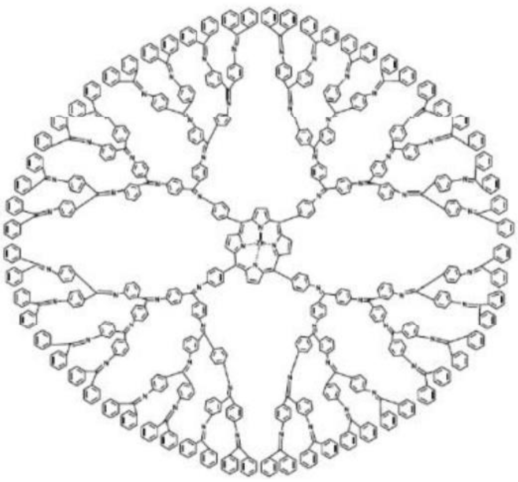

Figure 3. The molecular graph of DPZ_n

In the above structure, we obtain that $\{d(u),d(v): uv\in E(G_3)\}$ has four edge set partitions.

$d(u), d(v) \setminus uv\in E(G_3)$	(2, 2)	(2, 3)	(3, 3)	(3, 4)

Number of edges	$16\times2^n-4$	$40\times2^n-16$	$8\times2^n+12$	4

Table 3. Edge set partition of DPZ_n

We calculate the Gourava Sombor index of DPZ_n chemical graph as follows:

Theorem 9. Let G_3 be the chemical structure of DPZ_n. Then

$$GSO(G_3)=\left(64\sqrt{2}+40\sqrt{61}+24\sqrt{13}\right)2^n-16\sqrt{2}-16\sqrt{61}+36\sqrt{13}+4\sqrt{193}.$$

Proof: Applying definition and edge set partition of G_3, we conclude

$$GSO(G_3)=\sum_{uv\in E(G_3)}\left[\left(d(u)+d(v)\right)^2+\left(d(u)d(v)\right)^2\right]^{\frac{1}{2}}.$$

$$=\left(16\times2^n-4\right)\left[(2+2)^2+(2\times2)^2\right]^{\frac{1}{2}}+\left(40\times2^n-16\right)\left[(2+3)^2+(2\times3)^2\right]^{\frac{1}{2}}$$

$$+\left(8\times2^n+12\right)\left[(3+3)^2+(3\times3)^2\right]^{\frac{1}{2}}+4\left[(3+4)^2+(3\times4)^2\right]^{\frac{1}{2}}.$$

By solving the above equation, we obtain the desired result.

We calculate the reduced Gourava Sombor index of DPZ_n chemical graph as follows:

Theorem 10. Let G_3 be the chemical structure of DPZ_n.Then

$$RGSO(G_3)=\left(16\sqrt{5}+40\sqrt{13}+32\sqrt{2}\right)2^n-4\sqrt{5}-16\sqrt{13}+48\sqrt{2}+4\sqrt{61}.$$

Proof: Applying definition and edge set partition of G_3, we conclude

$$RGSO(G_3)=\sum_{uv\in E(G_3)}\left[\left(d(u)-1+d(v)-1\right)^2+\left((d(u)-1)(d(v)-1)\right)^2\right]^{\frac{1}{2}}.$$

$$=\left(16\times2^n-4\right)\left[(1+1)^2+(1\times1)^2\right]^{\frac{1}{2}}+\left(40\times2^n-16\right)\left[(1+2)^2+(1\times2)^2\right]^{\frac{1}{2}}$$

$$+\left(8\times2^n+12\right)\left[(2+2)^2+(2\times2)^2\right]^{\frac{1}{2}}+4\left[(2+3)^2+(2\times3)^2\right]^{\frac{1}{2}}.$$

By simplifying the above equation, we obtain the necessary result.

By using definitions and Table 3, we estalish the Gourava Sombor and reduced Gourava Sombor exponentials of DPZ_n chemical graph as follows:

Theorem 11. The Gourava Sombor exponential of DPZ_n is given by

$$GSO(G_3,x)=\left(16\times2^n-4\right)x^{4\sqrt{2}}+\left(40\times2^n-16\right)x^{\sqrt{61}}+\left(8\times2^n+12\right)x^{3\sqrt{13}}+4x^{\sqrt{193}}.$$

Theorem 12. The reduced Gourava Sombor exponential of DPZ_n is given by

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$$RGSO(G_3,x)=\left(16\times 2^n-4\right)x^{\sqrt{5}}+\left(40\times 2^n-16\right)x^{\sqrt{13}}+\left(8\times 2^n+12\right)x^{4\sqrt{2}}+4x^{\sqrt{61}}.$$

6. PORPHYRIN DENDRIMER D_nP_n

The chemical graphs G_4 of porphyrin dendrimers D_nP_n structure have $96n-10$ vertices and $105n-11$ edges are shown in Figure 4.

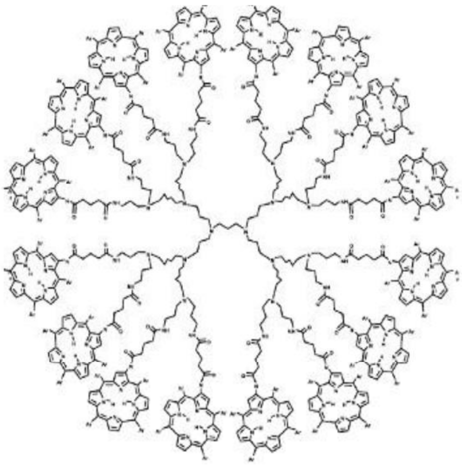

Figure 4. The molecular graph of D_nP_n

In the above structure, we obtain that $\{d(u),d(v): uv\in E(G_4)\}$ has six edge set partitions.

$d(u), d(v)\setminus uv\in E(G_4)$	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(3, 3)	(3, 4)
Number of edges	$2n$	$24n$	$10n-5$	$48n-6$	$13n$	$8n$

Table 4. Edge set partition of D_nP_n

We calculate the Gourava Sombor index of D_nP_n chemical graph as follows:

Theorem 13. Let G_4 be the chemical structure of D_nP_n. Then

$$GSO(G_4)=\left(10+24\sqrt{41}+40\sqrt{2}+48\sqrt{61}+39\sqrt{13}+8\sqrt{193}\right)n-20\sqrt{2}-6\sqrt{61}.$$

Proof: Applying definition and edge set partition of G_4, we conclude

$$GSO(G_4)=\sum_{uv\in E(G_4)}\left[\left(d(u)+d(v)\right)^2+\left(d(u)d(v)\right)^2\right]^{\frac{1}{2}}.$$

$$=2n\left[(1+3)^2+(1\times 3)^2\right]^{\frac{1}{2}}+24n\left[(1+4)^2+(1\times 4)^2\right]^{\frac{1}{2}}$$

$$+(10n-5)\left[(2+2)^2+(2\times 2)^2\right]^{\frac{1}{2}}+(48n-6)\left[(2+3)^2+(2\times 3)^2\right]^{\frac{1}{2}}$$

$$+13n\left[(3+3)^2+(3\times 3)^2\right]^{\frac{1}{2}}+8n\left[(3+4)^2+(3\times 4)^2\right]^{\frac{1}{2}}.$$

By solving the above equation, we obtain the desired result.

We calculate the reduced Gourava Sombor index of D_nP_n chemical graph as follows:

Theorem 14. Let G_4 be the chemical structure of D_nP_n .Then

$$RGSO(G_4)=\left(76+10\sqrt{5}+48\sqrt{13}+52\sqrt{2}+18\sqrt{41}\right)n-5\sqrt{5}-6\sqrt{13}.$$

Proof: Applying definition and edge set partition of G_4, we conclude

$$RGSO(G_4)=\sum_{uv\in E(G_4)}\left[\left(d(u)-1+d(v)-1\right)^2+\left((d(u)-1)(d(v)-1)\right)^2\right]^{\frac{1}{2}}$$

$$=2n\left[(0+2)^2+(0\times 2)^2\right]^{\frac{1}{2}}+24n\left[(0+3)^2+(0\times 3)^2\right]^{\frac{1}{2}}$$

$$+(10n-5)\left[(1+1)^2+(1\times 1)^2\right]^{\frac{1}{2}}+(48n-6)\left[(1+2)^2+(1\times 2)^2\right]^{\frac{1}{2}}$$

$$+13n\left[(2+2)^2+(2\times 2)^2\right]^{\frac{1}{2}}+8n\left[(2+3)^2+(2\times 3)^2\right]^{\frac{1}{2}}.$$

By simplifying the above equation, we obtain the necessary result.

By using definitions and Table 4, we get the Gourava Sombor and reduced Gourava Sombor exponentials of D_nP_n chemical graph as follows:

Theorem 15. The Gourava Sombor exponential of D_nP_n is given by

$$GSO(G_4,x)=2nx^5+24nx^{\sqrt{41}}+(10n-5)x^{4\sqrt{2}}+(48n-6)x^{\sqrt{61}}+13nx^{3\sqrt{13}}+8nx^{\sqrt{193}}.$$

Theorem 16. The reduced Gourava Sombor exponential of D_nP_n is given by

$$RGSO(G_4,x)=2nx^2+24nx^3+(10n-5)x^{\sqrt{5}}+(48n-6)x^{\sqrt{13}}+13nx^{4\sqrt{2}}+8nx^{\sqrt{41}}.$$

7. CONCLUSION

In this study, we have determined the Gourava Sombor index, the reduced Gourava Sombor index and their corresponding exponentials for some important dendrimers such as poly ethylene amide amine dendrimers, propyl ether imine dendrimers, zinc prophyrin dendrimers and porphyrin dendrimers which are appeared in nanoscience.

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