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IRREGULARITY DHARWAD INDICES OF CERTAIN NANOSTRUCTURES

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ABSTRACT

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

Keywords: *irregularity Dharwad index, irregularity reduced Dharwad index, nanostructure.*

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

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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 $d(u)$. For other graph terminologies and notions, the readers are referred to books [1, 2].

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 [3, 4].

In [5], the Dharwad index of a graph G was introduced and it is defined as

$$D(G)=\sum_{uv\in E(G)}\sqrt{d(u)^3+d(v)^3}.$$

Recently, some Dharwad indices were studied, for example, in [6, 7].

We introduce the irregularity Dharwad index of a graph G and it is defined as

$$ID(G)=\sum_{uv\in E(G)}\sqrt{\left|d(u)^3-d(v)^3\right|}.$$

We introduce the irregularity Dharwad exponential of a graph G and it is defined as

$$ID(G,x)=\sum_{uv\in E(G)}x^{\sqrt{\left|d(u)^3-d(v)^3\right|}}$$

Recently, some irregularity indices were studied, for example, in [8, 9. 10, 11, 12, 13, 14].

We also define the irregularity reduced Dharwad index of a graph G as

$$IRD(G)=\sum_{uv\in E(G)}\sqrt{\left|(d(u)-1)^3-(d(v)-1)^3\right|}.$$

Recently, some reduced indices were studied, for example, in [15, 16, 17, 18].

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We propose the irregularity reduced Dharwad exponential of a graph G and it is defined as

$$IRD(G,x)=\sum_{uv\in E(G)} x^{\sqrt{\left|(d(u)-1)^3-(d(v)-1)^3\right|}}$$

In this paper, the irregularity Dharwad index, the irregularity reduced Dharwad index and their corresponding exponential for certain nanostructures are determined.

2. RESULTS FOR POLY ETHYLENE AMIDE AMINE DENDRIMER *PETAA*

The chemical graphs G 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.

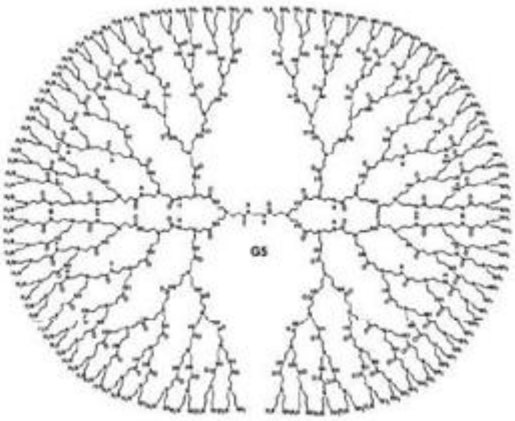

Figure-1: The molecular graph of *PETAA*

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

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

Table-1: Edge set partition of *PETAA*

We calculate the irregularity Dharwad index of *PETAA* chemical graph as follows:

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

$$ID(G)=\left(\sqrt{7}+\sqrt{26}+5\sqrt{19}\right)4\times2^n-2\sqrt{26}-9\sqrt{19}.$$

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

$$ID(G)=\sum_{uv\in E(G)}\sqrt{\left|d(u)^3-d(v)^3\right|}$$

$$=4\times2^n\sqrt{\left|1^3-2^3\right|}+\left(4\times2^n-2\right)\sqrt{\left|1^3-3^3\right|}$$

$$+\left(16\times2^n-8\right)\sqrt{\left|2^3-2^3\right|}+\left(20\times2^n-9\right)\sqrt{\left|2^3-3^3\right|}.$$

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

We calculate the irregularity Dharwad exponential of *PETAA* chemical graph as follows:

Theorem 2: The irregularity Dharwad exponential of *PETAA* is given by

$$ID(G,x)=\left(4\times2^n\right)x^{\sqrt{7}}+\left(4\times2^n-2\right)x^{\sqrt{26}}+\left(16\times2^n-8\right)x^{0}+\left(20\times2^n-9\right)x^{\sqrt{19}}.$$

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

$$ID(G,x)=\sum_{uv\in E(G)} x^{\sqrt{\left|d(u)^3-d(v)^3\right|}}$$

$$=\left(4\times2^n\right)x^{\sqrt{\left|1^3-2^3\right|}}+\left(4\times2^n-2\right)x^{\sqrt{\left|1^3-3^3\right|}}+\left(16\times2^n-8\right)x^{\sqrt{\left|2^3-2^3\right|}}$$

$$+\left(20\times2^n-9\right)x^{\sqrt{\left|2^3-3^3\right|}}.$$

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

We calculate the irregularity reduced Dharwad index of *PETAA* chemical graph as follows:

Theorem 3: Let *G* be the chemical structure of *PETAA*. Then

$$IRD(G)=\left(1+2\sqrt{2}+5\sqrt{7}\right)4\times 2^{n}-4\sqrt{2}-9\sqrt{7}.$$

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

$$IRD(G)=\sum_{uv\in E(G)}\sqrt{\left|\left(d(u)-1\right)^{3}-\left(d(v)-1\right)^{3}\right|}$$

$$=4\times 2^{n}\sqrt{\left|(1-1)^{3}-(2-1)^{3}\right|}+\left(4\times 2^{n}-2\right)\sqrt{\left|(1-1)^{3}-(3-1)^{3}\right|}$$

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

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

We calculate the irregularity reduced Dharwad exponential of *PETAA* chemical graph as follows:

Theorem 4: The irregularity Dharwad exponential of *PETAA* is given by

$$IRD(G,x)=\left(4\times 2^{n}\right)x^{\sqrt{7}}+\left(4\times 2^{n}-2\right)x^{\sqrt{26}}+\left(16\times 2^{n}-8\right)x^{0}+\left(20\times 2^{n}-9\right)x^{\sqrt{19}}.$$

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

$$IRD(G,x)=\sum_{uv\in E(G)}x^{\sqrt{\left|\left(d(u)-1\right)^{3}-\left(d(v)-1\right)^{3}\right|}}$$

$$=\left(4\times 2^{n}\right)x^{\sqrt{\left|(1-1)^{3}-(2-1)^{3}\right|}}+\left(4\times 2^{n}-2\right)x^{\sqrt{\left|(1-1)^{3}-(3-1)^{3}\right|}}$$

$$+\left(16\times 2^{n}-8\right)x^{\sqrt{\left|(2-1)^{3}-(2-1)^{3}\right|}}+\left(20\times 2^{n}-9\right)x^{\sqrt{\left|(2-1)^{3}-(3-1)^{3}\right|}}.$$

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

3. RESULTS FOR PROPYL ETHER IMINE DENDRIMER *PETIM*

The chemical graphs *H* 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.

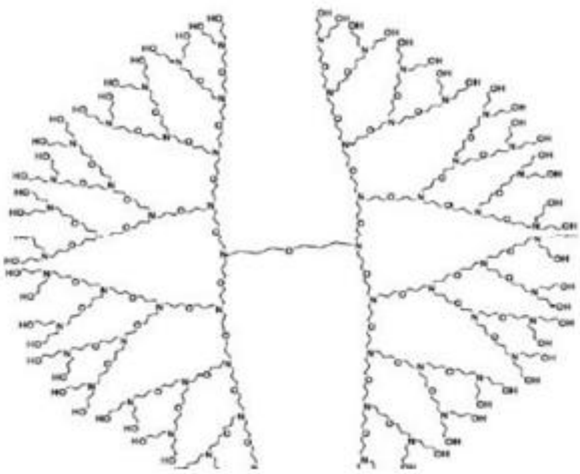

Figure-2: The molecular graph of *PETIM*

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

$d(u), d(v) \setminus uv \in E(H)$	(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 irregularity Dharwad index of *PETIM* chemical graph as follows:

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

$$ID(H)=\left(\sqrt{7}+3\sqrt{19}\right)2\times 2^{n}-6\sqrt{19}.$$

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

$$ID(H)=\sum_{uv\in E(H)}\sqrt{\left|d(u)^{3}-d(v)^{3}\right|}$$

$$=2\times 2^{n}\sqrt{\left|1^{3}-2^{3}\right|}+\left(16\times 2^{n}-18\right)\sqrt{\left|2^{3}-2^{3}\right|}+\left(6\times 2^{n}-6\right)\sqrt{\left|2^{3}-3^{3}\right|}.$$

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

We calculate the irregularity Dharwad exponential of *PETIM* chemical graph as follows:

Theorem 6: The irregularity Dharwad exponential of *PETIM* is given by

$$ID(H,x)=\left(2\times 2^{n}\right)x^{\sqrt{7}}+\left(16\times 2^{n}-18\right)x^{0}+\left(6\times 2^{n}-6\right)x^{\sqrt{19}}.$$

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

$$ID(H,x)=\sum_{uv\in E(H)}x^{\sqrt{\left|d(u)^{3}-d(v)^{3}\right|}}$$

$$=\left(2\times 2^{n}\right)x^{\sqrt{\left|1^{3}-2^{3}\right|}}+\left(16\times 2^{n}-18\right)x^{\sqrt{\left|2^{3}-2^{3}\right|}}+\left(6\times 2^{n}-6\right)x^{\sqrt{\left|2^{3}-3^{3}\right|}}.$$

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

We calculate the irregularity reduced Dharwad index of *PETIM* chemical graph as follows:

Theorem 7: Let *H* be the chemical structure of *PETIM.* Then

$$IRD(H)=\left(1+3\sqrt{7}\right)2\times 2^{n}-6\sqrt{7}.$$

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

$$IRD(H)=\sum_{uv\in E(H)}\sqrt{\left|\left(d(u)-1\right)^{3}-\left(d(v)-1\right)^{3}\right|}$$

$$=2\times 2^{n}\sqrt{\left|(1-1)^{3}-(2-1)^{3}\right|}+\left(16\times 2^{n}-18\right)\sqrt{\left|(2-1)^{3}-(2-1)^{3}\right|}$$

$$+\left(6\times 2^{n}-6\right)\sqrt{\left|(2-1)^{3}-(3-1)^{3}\right|}.$$

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

We calculate the irregularity reduced Dharwad exponential of *PETIM* chemical graph as follows:

Theorem 8: The irregularity Dharwad exponential of *PETIM* is given by

$$IRD(H,x)=\left(2\times 2^{n}\right)x^{1}++\left(16\times 2^{n}-18\right)x^{0}+\left(20\times 2^{n}-9\right)x^{\sqrt{7}}\left(4\times 2^{n}\right)x^{\sqrt{7}}.$$

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

$$IRD(H,x)=\sum_{uv\in E(H)}x^{\sqrt{\left|\left(d(u)-1\right)^{3}-\left(d(v)-1\right)^{3}\right|}}$$

$$=\left(2\times 2^{n}\right)x^{\sqrt{\left|(1-1)^{3}-(2-1)^{3}\right|}}+\left(16\times 2^{n}-18\right)x^{\sqrt{\left|(2-1)^{3}-(2-1)^{3}\right|}}+\left(6\times 2^{n}-6\right)x^{\sqrt{\left|(2-1)^{3}-(3-1)^{3}\right|}}.$$

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

4. RESULTS FOR ZINC PROPHYRIN DENDRIMER DPZ_n

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

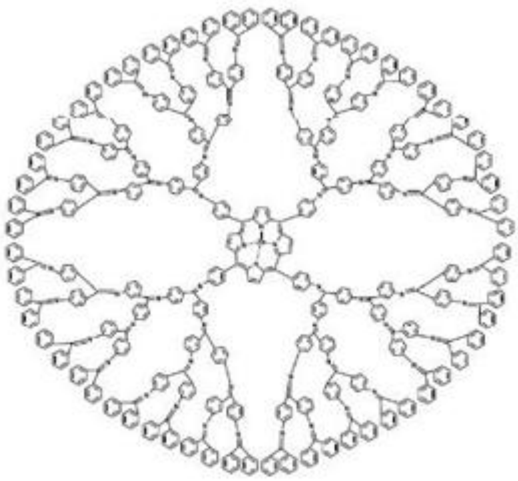

Figure-3: The molecular graph of DPZ_n

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

$d(u), d(v) \setminus uv \in E(K)$	(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 irregularity Dharwad index of DPZ_n chemical graph as follows:

Theorem 9: Let K be the chemical structure of DPZ_n. Then

$$ID(K) = 40\times 2^n\sqrt{19} - 16\sqrt{19} + 4\sqrt{37}.$$

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

$$ID(K) = \sum_{uv\in E(K)} \sqrt{\left|d(u)^3 - d(v)^3\right|}$$

$$= \left(16\times 2^n - 4\right)\sqrt{\left|2^3 - 2^3\right|} + \left(40\times 2^n - 16\right)\sqrt{\left|2^3 - 3^3\right|}$$

$$+\left(8\times 2^n + 12\right)\sqrt{\left|3^3 - 3^3\right|} + 4\sqrt{\left|3^3 - 4^3\right|}.$$

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

We calculate the irregularity Dharwad exponential of DPZ_n chemical graph as follows:

Theorem 10: The irregularity Dharwad exponential of DPZ_n is given by

$$ID(K,x) = \left(24\times 2^n + 8\right)x^0 + \left(40\times 2^n - 16\right)x^{\sqrt{19}} + 4x^{\sqrt{37}}.$$

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

$$ID(K,x) = \sum_{uv\in E(K)} x^{\sqrt{\left|d(u)^3 - d(v)^3\right|}}$$

$$= \left(16\times 2^n - 4\right)x^{\sqrt{\left|2^3-2^3\right|}} + \left(40\times 2^n - 16\right)x^{\sqrt{\left|2^3-3^3\right|}} + \left(8\times 2^n + 12\right)x^{\sqrt{\left|3^3-3^3\right|}} + 4x^{\sqrt{\left|3^3-4^3\right|}}.$$

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

We calculate the irregularity reduced Dharwad index of DPZ_n chemical graph as follows:

Theorem 11: Let K be the chemical structure of DPZ_n. Then

$$IRD(K) = 40\times 2^n\sqrt{7} - 16\sqrt{7} + 4\sqrt{19}.$$

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

$$IRD(K) = \sum_{uv\in E(K)} \sqrt{\left|\left(d(u)-1\right)^3 - \left(d(v)-1\right)^3\right|}$$

$$= \left(16\times 2^n - 4\right)\sqrt{\left|(2-1)^3-(2-1)^3\right|} + \left(40\times 2^n - 16\right)\sqrt{\left|(2-1)^3-(3-1)^3\right|}$$

$$+\left(8\times 2^n + 12\right)\sqrt{\left|(3-1)^3-(3-1)^3\right|} + 4\sqrt{\left|(3-1)^3-(4-1)^3\right|}.$$

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

We calculate the irregularity reduced Dharwad exponential of DPZ_n chemical graph as follows:

Theorem 12: The irregularity Dharwad exponential of DPZ_n is given by

$$IRD(K,x) = \left(24\times 2^n + 8\right)x^0 + \left(40\times 2^n - 16\right)x^{\sqrt{7}} + 4x^{\sqrt{19}}.$$

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

$$IRD(K,x) = \sum_{uv\in E(K)} x^{\sqrt{\left|\left(d(u)-1\right)^3-\left(d(v)-1\right)^3\right|}}$$

$$= \left(16\times 2^n - 4\right)x^{\sqrt{\left|(2-1)^3-(2-1)^3\right|}} + \left(40\times 2^n - 16\right)x^{\sqrt{\left|(2-1)^3-(3-1)^3\right|}}$$

$$+\left(8\times 2^n + 12\right)x^{\sqrt{\left|(3-1)^3-(3-1)^3\right|}} + 4x^{\sqrt{\left|(3-1)^3-(4-1)^3\right|}}.$$

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

5. RESULTS FOR PORPHYRIN DENDRIMER D_nP_n

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

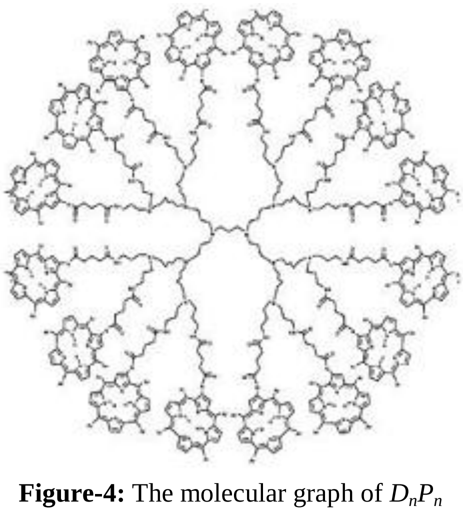

Figure-4: The molecular graph of D_nP_n

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

$d(u), d(v) \setminus uv \in E(D)$	(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 irregularity Dharwad index of D_nP_n chemical graph as follows:

Theorem 13: Let D be the chemical structure of D_nP_n. Then

$$ID(D) = \left(2\sqrt{26} + 24\sqrt{63} + 48\sqrt{19} + 8\sqrt{37}\right)n - 6\sqrt{19}.$$

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

$$\begin{aligned} ID(D) &= \sum_{uv\in E(D)} \sqrt{\left|d(u)^3 - d(v)^3\right|} \\ &= 2n\sqrt{\left|1^3 - 3^3\right|} + 24n\sqrt{\left|1^3 - 4^3\right|} + (10n-5)\sqrt{\left|2^3 - 2^3\right|} \\ &\quad + (48n-6)\sqrt{\left|2^3 - 3^3\right|} + 13n\sqrt{\left|3^3 - 3^3\right|} + 28n\sqrt{\left|3^3 - 4^3\right|}. \end{aligned}$$

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

We calculate the irregularity Dharwad exponential of D_nP_n chemical graph as follows:

Theorem 14: The irregularity Dharwad exponential of D_nP_n is given by

$$ID(D,x) = 2nx^{\sqrt{26}} + 24nx^{\sqrt{63}} + (23n-5)x^0 + (48n-6)x^{\sqrt{19}} + 8nx^{\sqrt{37}}.$$

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

$$\begin{aligned} ID(D,x) &= \sum_{uv\in E(D)} x^{\sqrt{\left|d(u)^3 - d(v)^3\right|}} \\ &= 2nx^{\sqrt{\left|1^3-3^3\right|}} + 24nx^{\sqrt{\left|1^3-4^3\right|}} + (10n-5)x^{\sqrt{\left|2^3-2^3\right|}} \\ &\quad + (48n-6)x^{\sqrt{\left|2^3-3^3\right|}} + 13nx^{\sqrt{\left|3^3-3^3\right|}} + 8nx^{\sqrt{\left|3^3-4^3\right|}}. \end{aligned}$$

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

We calculate the irregularity reduced Dharwad index of D_nP_n chemical graph as follows:

Theorem 15: Let D be the chemical structure of D_nP_n. Then

$$IRD(D) = \left(4\sqrt{2} + 72\sqrt{3} + 48\sqrt{7} + 8\sqrt{19}\right)n - 6\sqrt{7}.$$

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

$$\begin{aligned} IRD(D) &= \sum_{uv\in E(D)} \sqrt{\left|(d(u)-1)^3 - (d(v)-1)^3\right|} \\ &= 2n\sqrt{\left|(1-1)^3 - (3-1)^3\right|} + 24n\sqrt{\left|(1-1)^3 - (4-1)^3\right|} \\ &\quad + (10n-5)\sqrt{\left|(2-1)^3 - (2-1)^3\right|} + (48n-6)\sqrt{\left|(2-1)^3 - (3-1)^3\right|} \\ &\quad + 13n\sqrt{\left|(3-1)^3 - (3-1)^3\right|} + 8n\sqrt{\left|(3-1)^3 - (4-1)^3\right|}. \end{aligned}$$

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

We calculate the irregularity reduced Dharwad exponential of D_nP_n chemical graph as follows:

Theorem 16: The irregularity Dharwad exponential of D_nP_n is given by

$$IRD(D,x) = 2nx^{2\sqrt{2}} + 24nx^{3\sqrt{3}}(23n-5)x^0 + (48n-6)x^{\sqrt{7}} + 8nx^{\sqrt{19}}.$$

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

$$\begin{aligned} IRD(D,x) &= \sum_{uv\in E(D)} x^{\sqrt{\left|(d(u)-1)^3 - (d(v)-1)^3\right|}} \\ &= 2nx^{\sqrt{\left|(1-1)^3-(3-1)^3\right|}} + 24nx^{\sqrt{\left|(1-1)^3-(4-1)^3\right|}} \\ &\quad + (10n-5)x^{\sqrt{\left|(2-1)^3-(2-1)^3\right|}} + (48n-6)x^{\sqrt{\left|(2-1)^3-(3-1)^3\right|}} \\ &\quad + 13nx^{\sqrt{\left|(3-1)^3-(3-1)^3\right|}} + 8nx^{\sqrt{\left|(3-1)^3-(4-1)^3\right|}}. \end{aligned}$$

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

6. CONCLUSION

In this study, we have determined the irregularity Dharwad index, the irregularity reduced Dharwad 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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