International Journal of Engineering Sciences & Research Technology

(A Peer Reviewed Online Journal)
Impact Factor: 5.164

IJESRT

IJESRT
INTERNATIONAL JOURNAL OF ENGINEERING SCIENCES & RESEARCH TECHNOLOGY

IRREGULARITY NEIGHBORHOOD DHARWAD INDEX AND ITS EXPONENTIAL OF SOME NANOSTAR DENDRIMERS

V.R.Kulli
Department of Mathematics Gulbarga University, Gulbarga 585106, India.

ABSTRACT

In this paper, we introduce the irregularity neighborhood Dharwad index, irregularity neighborhood Dharwad exponential of a graph. Also we compute the irregularity neighborhood Dharwad index and its corresponding exponential for some important nanostructures which are appeared in nanoscience.

Keywords: irregularity neighborhood Dharwad index, irregularity neighborhood Dharwad exponential, dendrimer.
Mathematics Subject Classification: 05C05, 05C12, 05C35.

1. INTRODUCTION

Let $G = (V(G), E(G))$ be a finite, simple connected graph. A molecular graph is a simple graph related to the structure of a chemical compound. Each vertex of a molecular graph represents an atom of the molecule and its edges to the bonds between atoms. Let $s(u)$ denote the sum of the degrees of all vertices adjacent to a vertex u. For other undefined notations, readers may refer to [1, 2].

Chemical Graph Theory has an important effect on the development of Chemical Sciences. Topological index is a numerical parameter mathematically derived from the graph structure. Numerous topological indices have been considered in Theoretical Chemistry, especially in quantitative structure activity (*QSAR*) and quantitative structure property (*QSPR*) study, see [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].

The irregularity Dharwad index [7] of a graph G is

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

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

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

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

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

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

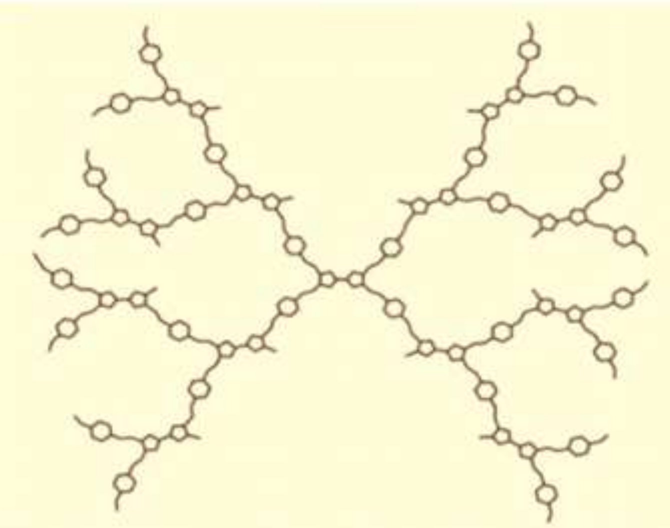
Recently, some neighborhood indices were studied, for example, in [15, 16, 17, 18, 19].

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

In this paper, we compute the irregularity neighborhood Dharwad index and irregularity neighborhood Dharwad exponential of tetrathiafulvalene, POPAM, $NS_2[n]$ and $NS_3[n]$ dendrimers.

2. TETRATHIAFULVALENE DENDRIMERS $TD_2[n]$

The molecular graph of tetrathiafulvalene dendrimers $TD_2[n]$ is shown in the below graph.



The graphs of $TD_2[n]$ have $31\times2^{n+2} - 74$ vertices and $35\times2^{n+2} - 85$ edges are shown in the above graph. Let $G= TD_2[n]$.

We obtain that $\{s(u), s(v): uv$ □ $E(G)\}$ has nine edge set partitions.

$s(u), s(v)\backslash uv$□$E(G)$	Number of edges
(2, 4)	2^{n+2}
(3, 6)	$2^{n+2} - 4$
(4, 6)	2^{n+2}
(5, 5)	$7\times2^{n+2} - 16$
(5, 6)	$11\times2^{n+2} - 24$
(5, 7)	$3\times2^{n+2} - 8$
(6, 6)	$2^{n+2} - 4$
(6, 7)	$8\times2^{n+2} - 24$
(7, 7)	$2\times2^{n+2} - 5$

Theorem 1. The irregularity neighborhood Dharwad index of $TD_2[n]$ is

$$IND(G) = \sqrt{56}\,2^{n+2} + \sqrt{185}\left(2^{n+2} - 4\right) + \sqrt{152}\,2^{n+2} + \sqrt{91}\left(11\times 2^{n+2} - 24\right).$$
$$+\sqrt{218}\left(3\times 2^{n+2} - 8\right) + \sqrt{127}\left(8\times 2^{n+2} - 24\right)$$

Proof: Applying definition and edge partition of $TD_2[n]$, we conclude

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

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

$$= 2^{n+2}\sqrt{|2^3-4^3|}+(2^{n+2}-4)\sqrt{|3^3-6^3|}+2^{n+2}\sqrt{|4^3-6^3|}+(7\times 2^{n+2}-16)\sqrt{|5^3-5^3|}$$
$$+(11\times 2^{n+2}-24)\sqrt{|5^3-6^3|}+(3\times 2^{n+2}-8)\sqrt{|5^3-7^3|}+(2^{n+2}-4)\sqrt{|6^3-6^3|}$$
$$+(8\times 2^{n+2}-24)\sqrt{|6^3-7^3|}+(2\times 2^{n+2}-5)\sqrt{|7^3-7^3|}$$

gives the desired result by solving the above equation.

Theorem 2. The irregularity neighborhood Dharwad exponential of $TD_2[n]$ iS

$$IND(G,x)=2^{n+2}x^{\sqrt{56}}+(2^{n+2}-4)x^{\sqrt{185}}$$
$$+2^{n+2}x^{\sqrt{152}}+(7\times 2^{n+2}-16)x^{0}+(11\times 2^{n+2}-24)x^{\sqrt{91}}+(3\times 2^{n+2}-8)x^{\sqrt{218}}$$
$$+(2^{n+2}-4)x^{0}+(8\times 2^{n+2}-24)x^{\sqrt{127}}+(2\times 2^{n+2}-5)x^{0}$$

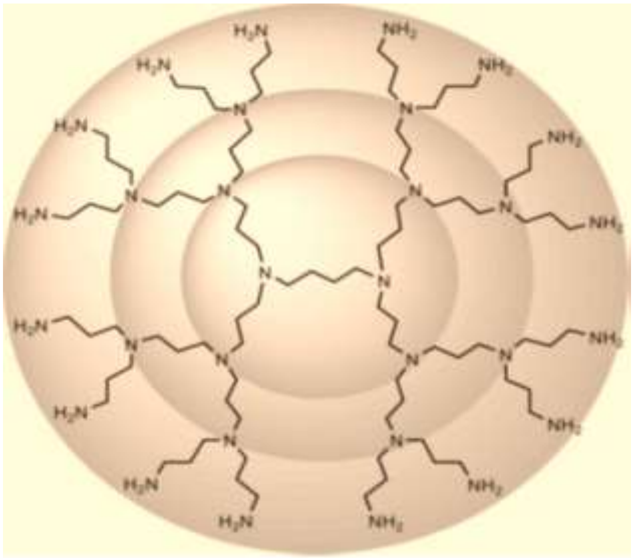
Proof: Applying definition and edge partition of $TD_2[n]$, we conclude

$$IND(G,x)=\sum_{uv\in E(G)} x^{\sqrt{|s(u)^3-s(v)^3|}}$$
$$=2^{n+2}x^{\sqrt{|2^3-4^3|}}+(2^{n+2}-4)x^{\sqrt{|3^3-6^3|}}+2^{n+2}x^{\sqrt{|4^3-6^3|}}+(7\times 2^{n+2}-16)x^{\sqrt{|5^3-5^3|}}$$
$$+(11\times 2^{n+2}-24)x^{\sqrt{|5^3-6^3|}}+(3\times 2^{n+2}-8)x^{\sqrt{|5^3-7^3|}}+(2^{n+2}-4)x^{\sqrt{|6^3-6^3|}}$$
$$+(8\times 2^{n+2}-24)x^{\sqrt{|6^3-7^3|}}+(2\times 2^{n+2}-5)x^{\sqrt{|7^3-7^3|}}$$

gives the desired result by solving the above equation.

3. POPAM DENDRIMERS $TD_2[n]$

The molecular graph of POPAM dendrimers $POD_2[n]$ is shown in the below graph.



The graphs of $POD_2[n]$ have $2^{n+5}-10$ vertices and $2^{n+5}-11$ edges are shown in the above graph. Let $B = POD_2[n]$.

We obtain that {*s(u), s(v): uv* □ *E(B)*} has five edge set partitions.

$s(u), s(v) \setminus uv$ □ $E(B)$	Number of edges
(2, 3)	2^{n+2}
(3, 4)	2^{n+2}
(4, 4)	1
(4, 5)	$3\times 2^{n+2} - 6$
(5, 6)	$3\times 2^{n+2} - 6$

Theorem 3. The irregularity neighborhood Dharwad index of $POD_2[n]$ is

$$IND(B) = \left(\sqrt{19}+\sqrt{37}+3\sqrt{61}+3\sqrt{91}\right)2^{n+2} - 6\left(\sqrt{61}+\sqrt{91}\right).$$

Proof: Applying definition and edge partition of $POD_2[n]$, we conclude

$$IND(B) = \sum_{uv\in E(B)} \sqrt{\left|s(u)^3 - s(v)^3\right|}$$

$$= 2^{n+2}\sqrt{\left|2^3-3^3\right|} + 2^{n+2}\sqrt{\left|3^3-4^3\right|} + 1\sqrt{\left|4^3-4^3\right|} + \left(3\times 2^{n+2}-6\right)\sqrt{\left|4^3-5^3\right|}$$

$$+\left(3\times 2^{n+2}-6\right)\sqrt{\left|5^3-6^3\right|}$$

gives the desired result by solving the above equation.

Theorem 4. The irregularity neighborhood Dharwad exponential of $POD_2[n]$ is

$$IND(B,x) = 2^{n+2}x^{\sqrt{19}} + 2^{n+2}x^{\sqrt{37}} + x^0 + \left(3\times 2^{n+2}-6\right)x^{\sqrt{61}} + \left(3\times 2^{n+2}-6\right)x^{\sqrt{91}}$$

Proof: Applying definition and edge partition of $POD_2[n]$, we conclude

$$IND(B,x) = \sum_{uv\in E(B)} x^{\sqrt{\left|s(u)^3-s(v)^3\right|}}$$

$$= 2^{n+2}x^{\sqrt{\left|2^3-3^3\right|}} + 2^{n+2}x^{\sqrt{\left|3^3-4^3\right|}} + 1x^{\sqrt{\left|4^3-4^3\right|}} + \left(3\times 2^{n+2}-6\right)x^{\sqrt{\left|4^3-5^3\right|}} + \left(3\times 2^{n+2}-6\right)x^{\sqrt{\left|5^3-6^3\right|}}$$

gives the desired result by solving the above equation.

4. $NS_2[n]$ DENDRIMERS

The molecular graph of $NS_2[n]$ dendrimers is shown in the below graph.

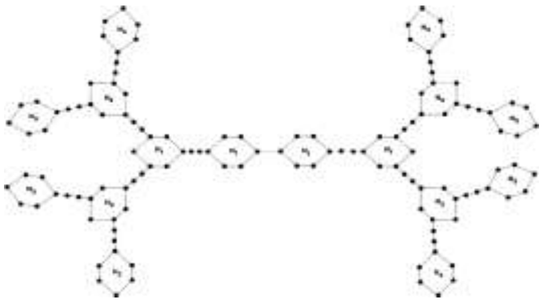


Figure 3. The molecular structure of $NS_2[3]$

The graphs of $NS_2[n]$ have $16\times 2^n - 4$ vertices and $18\times 2^n - 5$ edges are shown in the above graph. Let $C = NS_2[n]$.

We obtain that {*s(u), s(v): uv* □ *E(C)*} has five edge set partitions.

ISSN: 2277-9655
Impact Factor: 5.164
CODEN: IJESS7

$s(u), s(v)$ \ uv □ $E(C)$	Number of edges
(4, 4)	2×2^n
(5, 4)	2×2^n
(5, 5)	$2\times2^n+2$
(5, 6)	6×2^n
(7, 7)	1
(5, 7)	4
(6, 6)	$6\times2^n-12$

Theorem 5. The neighborhood Dharwad index of a $NS_2[n]$ dendrimer is

$$IND(C)=\left(\sqrt{61}+3\sqrt{91}\right)2\times2^n+4\sqrt{218}.$$

Proof: Applying definition and edge partition of $NS_2[n]$, we conclude

$$IND(C)=\sum_{uv\in E(C)}\sqrt{\left|s(u)^3-s(v)^3\right|}$$

$$=2\times2^n\sqrt{\left|4^3-4^3\right|}+2\times2^n\sqrt{\left|5^3-4^3\right|}+\left(2\times2^n+2\right)\sqrt{\left|5^3-5^3\right|}+6\times2^n\sqrt{\left|5^3-6^3\right|}$$

$$+1\sqrt{\left|7^3-7^3\right|}+4\sqrt{\left|5^3-7^3\right|}+\left(6\times2^n-12\right)\sqrt{\left|6^3-6^3\right|}$$

gives the desired result by solving the above equation.

Theorem 6. The irregularity neighborhood Dharwad exponential of $NS_2[n]$ is

$$IND(C,x)=\left(10\times2^n-9\right)x^0+2\times2^n x^{\sqrt{19}}+6\times2^n x^{\sqrt{91}}+4x^{\sqrt{218}}$$

Proof: Applying definition and edge partition of $NS_2[n]$ based on $S_G(u)$, $S_G(v)$, we conclude

$$IND(C,x)=\sum_{uv\in E(C)}x^{\sqrt{\left|s(u)^3-s(v)^3\right|}}$$

$$=2\times2^n x^{\sqrt{\left|4^3-4^3\right|}}+2\times2^n x^{\sqrt{\left|5^3-4^3\right|}}+\left(2\times2^n+2\right)x^{\sqrt{\left|5^3-5^3\right|}}+6\times2^n x^{\sqrt{\left|5^3-6^3\right|}}$$

$$+1x^{\sqrt{\left|7^3-7^3\right|}}+4x^{\sqrt{\left|5^3-7^3\right|}}+\left(6\times2^n-12\right)x^{\sqrt{\left|6^3-6^3\right|}}$$

gives the desired result by solving the above equation.

5. $NS_3[n]$ DENDRIMERS

The molecular graph of $NS_3[n]$ dendrimers is shown in the below graph.

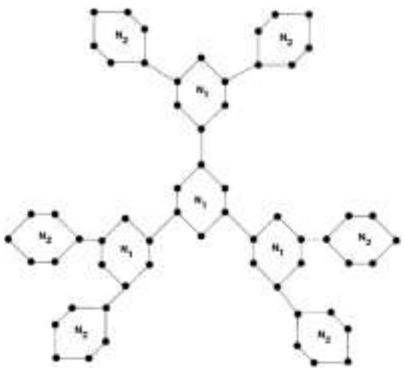


Figure 4. The molecular structure of NS_3[2]

The graphs of $NS_3[n]$ have $18\times2^n - 12$ vertices and $21\times2^n - 15$ edges are shown in the above graph. Let $D = NS_3[n]$.

We obtain that {*s(u), s(v): uv* □ *E(D)*} has five edge set partitions.

$s(u), s(v) \setminus uv$ □ $E(D)$	Number of edges
(4, 4)	3×2^n
(4, 5)	3×2^n
(5, 7)	3×2^n
(6, 7)	$9\times2^n - 12$
(7, 7)	$3\times2^n - 3$

Theorem 7. The irregularity neighborhood Dharwad index of $NS_3[n]$ is

$$IND(D) = \left(\sqrt{61} + \sqrt{218} + 3\sqrt{127}\right)3\times2^n - 12\sqrt{127}.$$

Proof: Applying definition and edge partition of $NS_3[n]$, we conclude

$$IND(D) = \sum_{uv\in E(D)} \sqrt{\left|s(u)^3 - s(v)^3\right|}$$

$$= 3\times2^n\sqrt{\left|4^3-4^3\right|} + 3\times2^n\sqrt{\left|4^3-5^3\right|} + 3\times2^n\sqrt{\left|5^3-7^3\right|} + \left(9\times2^n-12\right)\sqrt{\left|6^3-7^3\right|}$$

$$+\left(3\times2^n-3\right)\sqrt{\left|7^3-7^3\right|}$$

gives the desired result by solving the above equation.

Theorem 8. The irregularity neighborhood Dharwad exponential of $NS_3[n]$ is

$$IND(D,x) = \left(6\times2^n-3\right)x^0 + 3\times2^n x^{\sqrt{61}} + 3\times2^n x^{\sqrt{218}} + \left(9\times2^n-12\right)x^{\sqrt{127}}.$$

Proof: Applying definition and edge partition of $NS_2[n]$ based on $S_G(u)$, $S_G(v)$, we conclude

$$IND(D,x) = \sum_{uv\in E(D)} x^{\sqrt{\left|s(u)^3-s(v)^3\right|}}$$

$$= 3\times2^n x^{\sqrt{\left|4^3-4^3\right|}} + 3\times2^n x^{\sqrt{\left|4^3-5^3\right|}} + 3\times2^n x^{\sqrt{\left|5^3-7^3\right|}} + \left(9\times2^n-12\right)x^{\sqrt{\left|6^3-7^3\right|}}$$

$$+\left(3\times2^n-3\right)x^{\sqrt{\left|7^3-7^3\right|}}$$

gives the desired result by solving the above equation. .

6. CONCLUSION

In this paper, we have determined the irregularity neighborhood Dharwad index and irregularity neighborhood Dharwad exponential of certain dendrimers.

REFERENCES

1. V.R.Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India (2012).
2. F.Harary, *Graph Theory,Reading, Addison Wesley*, (1969).
3. S.Wagner and H.Wang, *Introduction Chemical Graph Theory*, Boca Raton, CRC Press, (2018).
4. M.V.Diudea (ed.) *QSPR/QSAR Studies by Molecular Descriptors*, NOVA New York, (2001).
5. V.R.Kulli, Dharwad indices, *International Journal of Engineering Sciences and Research Technology*, 10(4) (2021) 17-21.
6. K.Hamid et al, Topological analysis empowered bridge network variants by Dharwad indices, *Journal of Jilin University*, 41(10) (2022) 53-67.

7. V.R.Kulli, Irregularity Dharwad indices of certain nanostructures, submitted.
8. M.Albertson, The irregularity of a graph, *Ars Comb.* 46 (1997) 129-125.
9. W.Gao, H.Abdo and D.Dimitrov, On the irregularity of some molecular structures, *Can. J. Chem.* 95 (2017) 174-183.
10. I.Gutman, Topological indices and irregularity measures, *Bulletin of Society of Mathematicians*, 8 (2018) 469-475.
11. V.R.Kulli, New irregularity Nirmala indices of some chemical structures, *International Journal of Engineering Sciences and Research Technology*, 10(8) (2021) 33-42.
12. V.R.Kulli, New irregularity Sombor indices and new Adriatic (*a*, *b*)-*KA* indices of certain chemical drugs, *International Journal of Mathematics Trends and Technology*, 67(9) (2021) 105-113.
13. T.Reti, R.Sharfdini, A. Dregelyi-Kiss and H.Hagobin, Graph irregularity indices used as molecular discriptors in QSPR studies, *MATCH Commun. Math. Comput. Chem.* 79 (2018) 509-524.
14. B.Zhou and W.Luo, On irregularity of graphs, *ARS Comb.* 88 (2008) 55-64.
15. V.R.Kulli, Multiplicative *ABC, GA and AG* neighborhood Dakshayani indices of dendrimers, *International Journal of Fuzzy Mathematical Archive*, 17(2) (2019) 77-82.
16. V.R.Kulli, Neighborhood Nirmala index and its exponential of nanocones and dendrimers, *International Journal of Engineering Sciences and Research Technology*, 10(5) (2021) 47-56.
17. V.R.Kulli, Neighborhood Sombor index of some nanostructures, *International Journal of Mathematics Trends and Technology*, 67(5) (2021) 101-108.
18. V.R.Kulli, Neighborhood Sombor indices, *International Journal of Mathematics Trends and Technology*, 68(6) (2022) 195-204.
19. V.R.Kulli, Neighborhood sum atom bond connectivity indices of some nanostar demdrimers, *International Journal of Mathematics and Computer Research*, 11(2) (2023) 3230-3235.