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On Irregularity Indices for Fractal- and Cayley-Tree Type Dendrimers

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ABSTRACT

Consider $G = (V(G), E(G))$ as a simple connected (molecular) graph, whereas, $V(G)$ and $E(G)$ are the sets of vertices and edges, respectively. A graph is supposed to be regular if all vertices have equal degree, otherwise irregular. The fractal- and cayley-trees are irregular acyclic and connected graphs which are widely used to develop signal amplifiers for biosensors, cellular imaging and genetic engineering. The topological index (TI) serves as a mathematical function for determining numerical values of molecular graphs, aiding in the prediction of diverse physical, chemical, biological, thermodynamic, and structural properties. An irregular index, a specific type of TI, quantifies the irregularity of atomic bonding within chemical compounds represented by the graphs under analysis. This study focuses on calculating the irregularity indices for fractal dendrimers and Cayley tree-type dendrimers. A comparative analysis of the obtained indices is conducted using their numerical values and 3D visualizations. Lastly, the most efficient and consistent irregularity indices for fractal- and Cayley-tree dendrimers are identified and discussed.

Keywords: cayley-tree dendrimers, fractal dendrimers, irregularity indices, topological descriptors

1. INTRODUCTION

Graph theory is an evolving field that has become a central part of mathematics, playing a foundational role across multiple disciplines, including computer science, operations research, social networks, map colouring, chemical engineering, game theory, and mathematical chemistry. Specifically, chemical graph theory focuses on analyzing the physical and chemical properties, along with the structural characteristics, of chemical compounds. These properties include a variety of factors like temperature, heat of formation, weight, point of stability, freezing point, melting point, boiling point, solubility, heat formation, heat evaporation, and surface

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tension. By analyzing these characteristics, researchers can gain valuable insights into the behavior and composition of different compounds. For this purpose, while various mathematical tools and models are used in chemical graph theory, topological indices are most familiar [1].

Wiener [2] used a distance-based TI for the paraffins boiling point. [3] defined the novel indices for determining the total π-electron energy of alternant hydrocarbons. If all vertices in a graph have an identical degree, the graph is referred to as regular and vice versa. Irregularity indices are TIs that help us to characterize irregular graphs with various properties. [4] discussed graph irregularity indices as molecular descriptors of QSPR studies. [5] calculated irregularity indices for complex biomolecular networks. Bell [6] defined different novel properties for irregularity of graphs. Gutman [7] determined and discussed the Irregularity of quasi perfect molecular graphs. Majcher et al. [8] discussed highly irregular graphs with an extreme number of edges. Liu et al. [9] calculated maximally irregular triangle free graphs and size of maximally irregular graphs. [10-12] investigated the change of the total irregularity of graphs under various subdivision operations.

Zahid et al. [13] analyzed irregularity measures of particular nanotubes, as observed by Gao et al. [14] calculated irregularity of indices of some molecular graphs of various classes of dendrimers. Imbalance-based irregularity indices of boron nanotubes were computationally analyzed [15]. Dimitrov et al. [16] discussed graphs with equal irregularity indices. The irregularity of indices has been concentrated as of late in a novel manner [9, 17]. The irregularity of such as $AL(G)$, irregularity index $IRL(G)$ and $IRLU(G)$ is imported as in the previous study presented by Albertson [18]. Other indices handled the concept of imbalance of an edge discussed [19].

Gutman et al. [20] gave new idea of the $IRF(G)$ irregularity index for graphs. Imran et al. [21] worked on fractal- and cayley-tree type dendrimers and calculated various irregularity indices for these graphs. Manimaran utilized edge partition method to investigate Sombor variants for tree Graph, Fractal-, and Cayley-Tree Type Dendrimers [22]. Hamanakaet al. [23] assessed non-Hermitian skin effect on the cayley tree through multifractal statistics. Pannipitiya investigated a dynamical approach to the Potts model on cayley tree [24]. FDEs attracted significant consideration due to their ability to model composite phenomena, such as visco-elastic materials [25], economics [26], continuum and statistical mechanics [27].

Fractal dendrimer is denoted by F_q and constructed from F_{q-1} by performing some steps at first to make a way of three connections with two same end nodes. After that, r new nodes are made for every one of the two center nodes of F_{q-1} and then they are attached to the center nodes. Cayley tree dendrimer is denoted by $C_{p,q}$ and obtained from $C_{p,q-1}$ by performing $p-1$ and vertices are generated and attached to the boundary vertices.

The following study unfolds as under: Section 2 covers preliminary information. Section 3 covers irregularity indices for fractal-trees, while Section 4 explores irregularity indices for cayley trees. The paper concludes in Section 5.

2. PRELIMINARIES

Suppose $G = (V(G), E(G))$ is a simple connected graph, where $V(G)$ & $E(G)$ are sets of vertices & edges, respectively. Whereas, the total number of edges adjacent to any vertex n_i is called degree of the vertex, which is denoted as $d(n_i)$. A graph is considered connected if there is always a path connecting every pair of vertices within the graph. Connected and acyclic graph is called a tree. In tree the vertices that have $d(v) \geq 3$ is the branching point. A tree-graph is chemical tree has $\Delta(G) = 4$. Any graph is supposed to be a regular graph if all of its vertices have a similar degree. The majority of Irregularity indices are from the family of degree based topological lists and are utilized in quantitative structure action relationship demonstrating.

Table 1. Irregularity Indices

Irregularity Indices	Mathematical Demonstration	Reference
imball $_{uv}$	$\lvert d_u - d_v \rvert$	[21]
AL（G)	$\sum_{n_1 n_2 \in E(G)} \lvert d(n_1) - d(n_2) \rvert$	[22]
$IRL(G)$	$\sum_{n_1 n_2 \in E(G)} \lvert lnd(n_1) - ln\ d(n_2) \rvert$	[22]

Irregularity Indices	Mathematical Demonstration	Reference
$IRR_t\,(G)$	$\frac{1}{2}\sum_{n_1n_2\in E(G)} \lvert d_G(n_1)-d_G(n_2)\rvert$	[11]
$IRF(G)$	$\sum_{n_1n_2\in E(G)} \left(d_G(n_1)-d_G(n_2)\right)^2$	[20]
$IRA(G)$	$\sum_{n_1n_2\in E(G)} \left(\frac{1}{\sqrt{d(n_1)}}-\frac{1}{\sqrt{d(n_2)}}\right)^2$	[4]
$IRDIF(G)$	$\sum_{n_1n_2\in E(G)} \left(\left\lvert\frac{d(n_1)}{d(n_2)}-\frac{d(n_2)}{d(n_2)}\right\rvert\right)$	[4]
$IRLF(G)$	$\sum_{n_1n_2\in E(G)} \frac{\lvert d_G(n_1)-d_G(n_2)\rvert}{d(n_1)d(n_2)}$	[4]
LA(G)	$2\sum_{n_1n_2\in E(G)} \frac{\lvert d_G(n_1)-d_G(n_2)\rvert}{d(n_1)+d(n_2)}$	[4]
$IRLF(G)$	$\sum_{n_1n_2\in E(G)} \frac{\lvert d_G(n_1)-d_G(n_2)\rvert}{\sqrt{\left(d(n_2)d(n_1)\right)}}$	[4]
IRD1(G)	$\sum_{n_1n_2\in E(G)} ln\ 1+\left\lvert d_{n_1}+d_{n_2}\right\rvert$	[4]
$IRGA(G)$	$\sum_{n_1n_2\in E(G)} ln\ \frac{d_{n_1}+d_{n_2}}{2\left(\sqrt{d_{n_1}d_{n_2}}\right)}$	[4]

Irregularity Indices	Mathematical Demonstration	Reference
$IRLU(G)$	$\frac{\sum_1 \underline{n_2 \in E(G)}\, ln\ d(n_1) - ln\ d(r}{min\big(d(n_1)d(n_1)\big)}$	[4]
$IRB(G)$	$\sum_{n_1 n_2 \in E(G)} \left(\sqrt{d_{n_1}} - \sqrt{d_{n_2}}\right)^2$	[4]

3. IRREGULARITY INDICES FOR FRACTAL-TREE DENDRIMERS

The term fractal is derived from Latin signifying "to break", and graph designs in that each littler piece of the structure is like as entirety. There are numerous instances of fractal dendrimers, such as broccoli, sierpinski triangle, lotus white flower, von koch curve, , ferns etc. This work explores the proposed fractal-tree dendrimers for F_q where $q \geq 0$ is the repetition if $q = 0$ then F_0 only an edge connecting two exact nodes. F_q is borrowed from F_{q-1} while performing three operations in every edge of F_{q-1}.

- Step 1 to make a way of three connections with two same end nodes.
- Step 2 to make r new nodes for every one of the two center nodes.
- Step 3 attached all r new nodes to the center nodes.

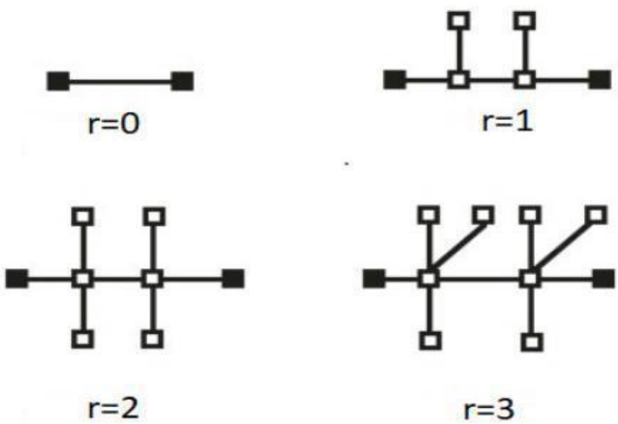


Figure 1. Fractal-tree Dendrimer F_0.

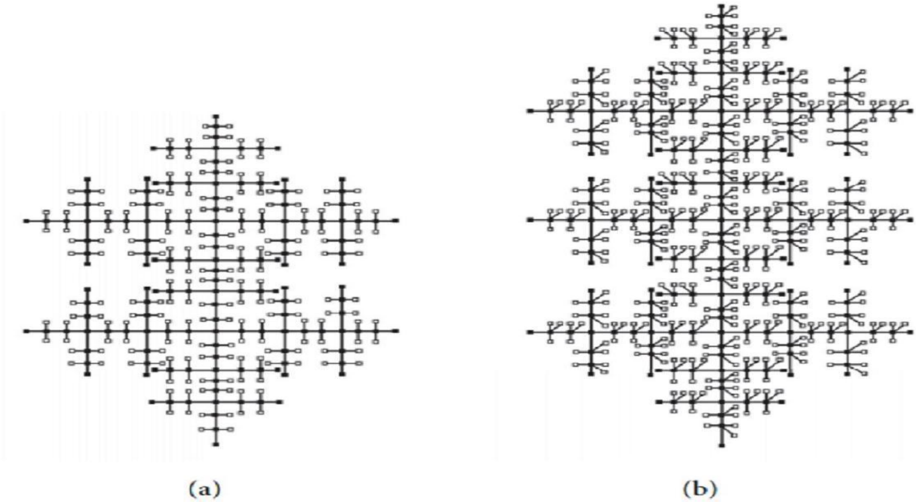


Figure 2. Fractal-tree Dendrimer (a) F_3 and $r = 2$ and (b) F_4 and $r = 3$

Table 2. Separation of Edge Set of Fractal-Tree Dendrimer Based on Degrees of End Vertices

$d(n_1), d(n_1)$	$(r+2, r+2)$	$(4, r+2)$	$(1, r+2)$
No. of edges	$21q - 14$	$28q - 20$	$42rq + 14q - 28r - 8$

Theorem 1. Let $G \cong F_q$ be a Fractal-Tree dendrimer then its irregularity indices are given as

(i) $IRR(G) = (42rq + 14q - 28r - 8)| - (r+1)| + (28q - 20)| - r + 2|$.

(ii) $IRL(G) = (42kp + 14p - 28k - 8)(ln\,(r+2)) + (28q - 20)ln\left(\frac{4}{r+2}\right)$.

(iii) $IRR_t(G) = \frac{1}{2}[(42rq + 14q - 28r - 8)| - (r+1)| + (28q - 20)| - r + 2|]$.

(iv) $IRF(G) = (42rq + 14q - 28r - 8)(-r-1)^2 + (28q - 20)(-r + 2)^2$.

(v) $IRD1 = (42rq + 14q - 28r - 8)(ln\,(1 + | - r - 1|)) + (28q - 20)(ln\,(1 + | - r + 2|))$.

(vi) $IRB(G) = \left[(42rq + 14q - 28r - 8)(1 - \sqrt{r+2})^2\right] + \left[(28q - 20)(2 - \sqrt{r+2})^2\right].$

Proof:

(i) $IRR(G) = \sum_{n_1 n_2 \in E(G)} |d_G(n_1) - d_G(n_2)|$

$$= \left[\sum_{n_1 n_2 \in E_{1,r+2}} + \sum_{n_1 n_2 \in E_{4,r+2}} + \sum_{n_1 n_2 \in E_{r+2,r+2}}\right] |d_G(n_1) - d_G(n_2)|$$

$$= (42rq + 14q - 28r - 8)|d_G(n_1) - d_G(n_2)| + (28q - 20)|d_G(n_1) - d_G(n_2)| \quad + 21q - 14|d_G(n_1) - d_G(n_2)|$$

$$= (42rq + 14q - 28r - 8)|d_G(n_1) - d_G(n_2)| + (28q - 20)|d_G(n_1) - d_G(n_2)|$$

$$= (42rq + 14q - 28r - 8)|1 - r - 2| + (28q - 20)|4 - r - 2|$$

$$= (42rq + 14q - 28r - 8)|-(r+1)| + (28q - 20)|-r + 2|$$

(ii) $IRL(G) = \sum_{n_1 n_2 \in E(G)} |lnd(n_1) - lnd(n_2)|$

$$= \left[\sum_{n_1 n_2 \in E_{1,r+2}} + \sum_{n_1 n_2 \in E_{4,r+2}} + \sum_{n_1 n_2 \in E_{r+2,r+2}}\right] |lnd(n_1) - ln\ d(n_2)|$$

$$= (42rq + 14q - 28r - 8)|ln\,(1) - ln\,(r+2)| + (28q - 20)|ln\,(4) - ln\,(r+2)| \quad + (21q - 14)|ln\,(r+2) - ln\,(r+2)|$$

$$= (42rq + 14q - 28r - 8)(ln\,(r+2)) + (28q - 20) ln\, \frac{4}{r+2}$$

(iii) $IRR_t(G) = \frac{1}{2} \sum_{n_1 n_2 \in E(G)} |d_G(n_1) - d_G(n_2)|$

$$= \frac{1}{2}\left[\sum_{n_1 n_2 \in E_{1,r+2}} + \sum_{n_1 n_2 \in E_{4,r+2}} + \sum_{n_1 n_2 \in E_{r+2,r+2}}\right] [|d_G(n_1) - d_G(n_2)|]$$

$$= \frac{1}{2}[(42rq + 14q - 28r - 8)|d_G(n_1) - d_G(n_2)| + (28q - 20)|d_G(n_1) - d_G(n_2)| \quad + 21q - 14|d_G(n_1) - d_G(n_2)|]$$

$$= \frac{1}{2}[(42rq + 14q - 28r - 8)|-(r+1)| + (28q - 20)|-r + 2|]$$

(iv) $IRF(G) = \sum_{n_1 n_2 \in E(G)} \left(d_G(n_1) - d_G(n_2)\right)^2$

$$= \left[\sum_{n_1 n_2 \in E_{1,r+2}} + \sum_{n_1 n_2 \in E_{4,r+2}} + \sum_{n_1 n_2 \in E_{r+2,r+2}}\right] \left(d_G(n_1) - d_G(n_2)\right)^2$$

$$= (42rq + 14q - 28r - 8)\left(d_G(n_1) - d_G(n_2)\right)^2 + (28q - 20)\left(d_G(n_1) - d_G(n_2)\right)^2 + (21q - 14)\left(d_G(n_1) - d_G(n_2)\right)^2$$

$$= (42rq + 14q - 28r - 8)(1 - r - 2)^2 + (28q - 20)(4 - r - 2)^2$$

$$= (42rq + 14q - 28r - 8)(-r - 1)^2 + (28r - 20)(-k + 2)^2$$

(v) $IRD1(G) = \sum_{n_1 n_2 \in E(G)} \left(ln\ (1 + |d_G(n_1) + d_G(n_2)|)\right)$

$$= \left[\sum_{n_1 n_2 \in E_{1,r+2}} + \sum_{uv \in E_{4,r+2}} + \sum_{uv \in E_{r+2,r+2}}\right] (\ln(1 + |d_G(n_1) + d_G(n_2)|))$$

$$= (42rq + 14q - 28r - 8)\left(ln\ (1 + |d_u + d_v|)\right) + (28q - 20)\left(ln\ (1 + |d_u + d_v|)\right) + (21q - 14)\left(ln\ (1 + |d_u + d_v|)\right)$$

$$= (42rq + 14q - 28r - 8)(ln\ (1 + |-r - 1|)) + (28q - 20)(ln\ (1 + |-r + 2|)) \quad + 21q - 14(ln\ (1 + |r + 2 - r - 2|))$$

$$= (42rq + 14q - 28r - 8)(ln\ (1 + |-r - 1|)) + (28q - 20)(ln\ (1 + |-r + 2|))$$

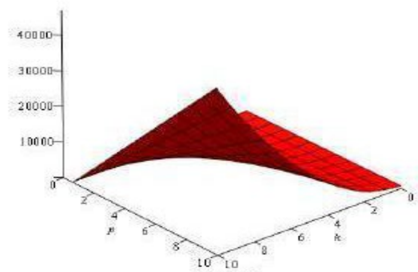
(vi) $IRB(G) = \sum_{n_1 n_2 \in E(G)} \left(\sqrt{d_{n_1}} - \sqrt{d_{n_2}}\right)^2$

$$= \left[\sum_{n_1 n_2 \in E_{1,r+2}} + \sum_{n_1 n_2 \in E_{4,r+2}} + \sum_{n_1 n_2 \in E_{r+2,r+2}}\right] \left(\sqrt{d_u} - \sqrt{d_v}\right)^2$$

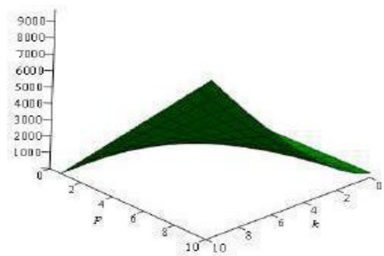
$$= (42rq + 14q - 28r - 8)\left(\sqrt{d_{n_1}} - \sqrt{d_{n_2}}\right)^2 + (28q - 20)\left(\sqrt{d_{n_1}} - \sqrt{d_{n_2}}\right)^2$$
$$+ (21q - 14)\left(\sqrt{d_{n_1}} - \sqrt{d_{n_2}}\right)^2$$
$$= (42rq + 14q - 28r - 8)(\sqrt{1} - \sqrt{r+2})^2 + (28q - 20)(\sqrt{4}$$
$$- \sqrt{r+2})^2 \quad + 21q - 14(\sqrt{r+2} - \sqrt{r+2})^2$$
$$= \left[(42rq + 14q - 28r - 8)(1 - \sqrt{r+2})^2\right]$$
$$+ \left[(28q - 20)(2 - \sqrt{r+2})^2\right]$$

Table 3. Irregularity Indices Related to Theorem 1

r, q	IRL(G)	IRR(G)	$IRR R_t(G)$	IRF(G)	IRD1	IRB(G)
(1,1)	24.2737	48	24	88	27.5174	11.2923
(1,2)	93.8510	188	94	340	108.4478	43.3129
(1,3)	163.42	328	164	592	189.3782	75.33
(1,4)	232.99	468	234	844	270.3086	107.34
(1,5)	302.58	608	304	1096	351.23	139.36
(1,6)	372.15	748	374	1348	432.16	171.38
(1,7)	441.7380	888	444	1600	513.09	203.4
(1,8)	511.3	1028	514	1852	594.02	235.43
(1,9)	580.89	1168	584	2104	674.96	267.45
(1,10)	650.46	1308	654	2356	755.88	299.47
(1,11)	720.04	1448	724	2608	836.81	331.49
(1,12)	789.61	1588	794	2860	897.74	363.51
(1,13)	859.19	1784	864	3112	998.67	395.53
(1,14)	928.77	1868	934	3364	1079.61	427.55
(1,15)	998.35	2008	1004	3661	1160.53	459.57
(1,16)	1067.92	2148	1074	3868	1241.46	491.59
(1,17)	11137.5	2288	1144	4120	1322.39	523.61
(1,18)	1229.85	2428	1214	4372	1403.33	555.63
(1,19)	1276.66	2568	1284	4624	1484.26	587.65
(1,20)	1346.23	2708	1354	4876	1565.18	619.68



$irr(G)$



$IRL(G)$

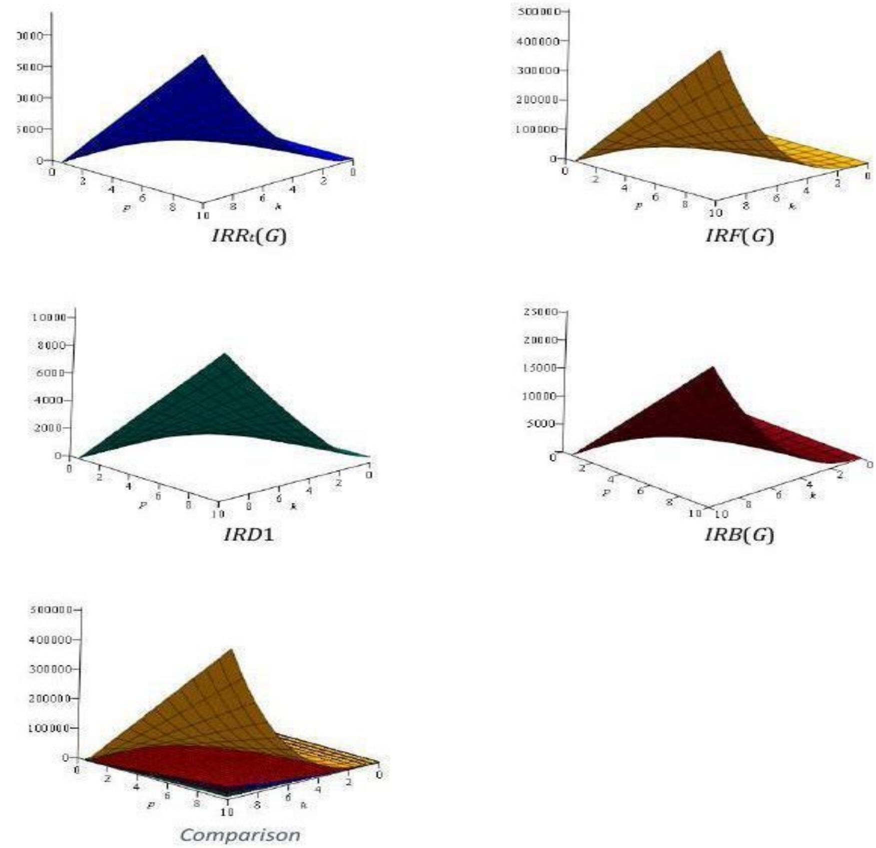


Figure 3. Comparison of the Irregularity Indices indicated with distinct colors *i.e.*, IRR( )by red color , IRL( )by green color, IRR_t( )by blue color, IRF( )by yellow color, IRD1( )by dark green color and IRB( ) by Plum Color

Among these indices $IRR(G)$ is a more dominant irregularity index for fractal-tree dendrimers.

Theorem 2. Let $G \cong F_q$ be a Fractal-Tree dendrimer then its irregularity indices are given as

(i) $IRLU(G) = (42rq + 14q - 28r - 8)\left(\frac{|-(r+1)|}{1}\right) + (28q - 20)\left(\frac{|-r+2|}{r+2}\right)$.

(ii) $IRLU(G) = (42rq + 14q - 28r - 8)\frac{|-(r+1)|}{1} + (28q - 20)\frac{|-r+2|}{4}$.

(iii) $IRA(G) = \frac{1}{r+2}\Big[(42rq + 14q - 28r - 8)(\sqrt{r+2} - 1)^2 + \left(\frac{28q-20}{4}\right)(\sqrt{r+2} - 2)^2\Big]$.

(iv) $IRDIF(G) = (42rq + 14q - 28r - 8)\left(\left|\frac{-r-1}{r+2}\right|\right) + (28q - 20)\left(\left|\frac{-r+2}{r+2}\right|\right)$.

(v) $IRLF(G) = \frac{1}{r+2}\Big[(42rq + 14q - 28r - 8)|-r-1| + (28q - 20)\frac{|-r+2|}{4}\Big]$.

(vi) $LA(G) = 2[(42rq + 14q - 28r - 8)\left(\frac{|-r-1|}{r+3}\right) + (28q - 20)\left(\frac{|-r-2|}{r+6}\right)$.

(vii) $IRGA(G) = (42rq + 14q - 28r - 8)\left(ln\ \frac{r+3}{2(\sqrt{r+2})}\right) + (28q - 20)(ln\ \frac{r+6}{2(\sqrt{4(r+2)})} + (21q - 14)(ln\ (2))$.

Proof:

(i) $IRLU(G) = \sum_{uv\in E(G)} \frac{|lnd_G(n_1) - lndd_G(n_2)|}{min(d(n_1),d(n_2))}$

$$= \left[\sum_{uv\in E_{1,r+2}} + \sum_{uv\in E_{r+2,r+2}} + \sum_{uv\in E_{r+2,r+2}}\right]\frac{|lndd_G(n_1) - lndd_G(n_2)|}{min(d(n_1),d(n_2))}$$

$$= (42rq + 14q - 28r - 8)\frac{|lnd(n_1) - lnd(n_2)|}{min(d(n_1),d(n_2))} + (28q - 20)\frac{|lnd(u) - lnd(v)|}{min(d(n_1),d(n_2))} + (21q - 14)\frac{|lnd(n_1) - lnd(n_2)|}{min(d(n_1),d(n_2))}$$

$$= (42rq + 14q - 28r - 8))\frac{|1 - r - 2|}{1} + (28q - 20)\frac{|4 - r - 2|}{k + 2} + (21q - 14)\left(\frac{|r + 2 - r - 2|}{r + 2}\right)$$

$$= (42rq + 14q - 28r - 8)\left(\frac{|-(r + 1)|}{1}\right) + (28q - 20)\left(\frac{|r + 2|}{r + 2}\right)$$

or

(ii) $IRLU(G) = \sum_{n_1 n_2 \in E(G)} \frac{|ln\ d_G(n_1) - ld_G(n_2)|}{min(d(n_1), d(n_2))}$

$$= \left[\sum_{n_1 n_2 \in E_{1,r+2}} + \sum_{n_1 n_2 \in E_{4,r+2}} + \sum_{n_1 n_2 \in E_{r+2,r+2}}\right] + \frac{|lnd\ \ _G(n_1) - ln\ d_G(n_2)|}{min(d(n_1), d(n_2))} =$$

$$= [(42rq + 14q - 28r - 8) + (28q - 20) + (21q - 14)]\frac{|ln\ d_G(n_1) - lndd_G(n_2)|}{min(d(n_1), d(n_2))}$$

$$= (42rq + 14q - 28r - 8)\left(\frac{|1 - r - 2|}{1}\right) + (28q - 20)\left(\frac{|4 - r - 2|}{4}\right) + (21q - 14)\left(\frac{|r + 2 - r - 2|}{r + 2}\right)$$

$$= (42rq + 14q - 28r - 8)\left(\frac{|-(r + 1)|}{1}\right) + (28q - 20)\left(\frac{|-r + 2|}{4}\right)$$

(iii) $IRA(G) = \sum_{n_1 n_2 \in E(G)} \left(\frac{1}{\sqrt{d(n_1)}} - \frac{1}{\sqrt{d(n_2)}}\right)^2$

$$= \left[\sum_{n_1 n_2 \in E_{1,r+2}} + \sum_{n_1 n_2 \in E_{4,r+2}} + \sum_{n_1 n_2 \in E_{r+2,r+2}}\right]\left(\frac{1}{\sqrt{d(n_1)}} - \frac{1}{\sqrt{d(n_2)}}\right)^2$$

$$= [(42rq + 14q - 28r - 8) + (28q - 20) + (21q - 14)]\left(\frac{1}{\sqrt{d(n_1)}} - \frac{1}{\sqrt{d(n_2)}}\right)^2$$

$$= (42rq + 14q - 28r - 8)\left(\frac{1}{\sqrt{1}} - \frac{1}{\sqrt{r+2}}\right)^2 + (28q - 20)\left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{r+2}}\right)^2 + (21q - 14)\left(\frac{1}{\sqrt{4}} - \frac{1}{\sqrt{r+2}}\right)^2$$

$$= \frac{1}{r+2}\left[(42rq + 14q - 28r - 8)(\sqrt{r+2} - 1)^2 + \frac{(28q - 20)}{4}(\sqrt{r+2} - 2)^2\right]$$

(iv) $IRDIF(G) = \sum_{n_1 n_2 \in E(G)} \left(\left|\frac{d(n_1)}{d(n_2)} - \frac{d(n_2)}{d(n_2)}\right|\right)$

$$= \left[\sum_{n_1 n_2 \in E_{1,r+2}} + \sum_{n_1 n_2 \in E_{4,r+2}} + \sum_{n_1 n_2 \in E_{r+2,r+2}}\right]\left(\left|\frac{1}{r+2} - \frac{r+2}{r+2}\right|\right)$$

$$= (42rq + 14q - 28r - 8)\left(\left|\frac{1}{k+2} - \frac{r+2}{r+2}\right|\right) + (28q - 20)\left(\left|\frac{1}{r+2} - \frac{r+2}{r+2}\right|\right) + (21q - 14)\left(\left|\frac{1}{r+2} - \frac{r+2}{r+2}\right|\right)$$

$$= (42rq + 14q - 28r - 8)\left(\left|\frac{1}{r+2} - \frac{r+2}{r+2}\right|\right) + (28q - 20)\left(\left|\frac{4}{r+2} - \frac{r+2}{r+2}\right|\right) + (21q - 14)\left(\left|\frac{r+2}{r+2} - \frac{r+2}{r+2}\right|\right)$$

$$= (42rq + 14q - 28r - 8)\left(\left|\frac{-r-1}{r+2}\right|\right) + q(28q - 20)\left(\left|\frac{-r+2}{r+2}\right|\right)$$

(v) $IRLF(G) = \sum_{n_1 n_2 \in E(G)} \frac{|d_G(n_1) - d_G(n_2)|}{\sqrt{(d(n_1)d(n_2))}}$

$$= \left[\sum_{n_1n_2 \in E_{1,r+2}} + \sum_{n_1n_2 \in E_{4,r+2}} + \sum_{n_1n_2 \in E_{r+2,r+2}} \right] \frac{|d_G(n_1) - d_G(n_2)|}{\sqrt{(d(v)d(u))}}$$

$$= (42rq + 14q - 28r - 8) \frac{|d_G(n_1) - d_G(n_2)|}{\sqrt{(d(n_2)d(n_1))} + (28q - 20) \frac{|d_G(n_1) - d_G(n_2)|}{\sqrt{(d(n_2)d(n_1))}} + (21q - 14) \frac{|d_G(n_1) - d_G(n_2)|}{\sqrt{(d(n_2)d(n_1))}}}$$

$$= (42rq + 14q - 28r - 8) \frac{|1 - r - 2|}{r+2} + (28q - 20) \frac{|4 - r - 2|}{4(r+2)} + (21q - 14) \frac{|r + 2 - r - 2|}{(r+2)(r+2)}$$

$$= \frac{1}{r+2} \left[(42rq + 14q - 28r - 8)| - r - 1| + (28q - 20) \frac{| - r + 2|}{4} \right]$$

(vi) $LA(G) = 2\sum_{n_1n_2 \in E(G)} \frac{|dd_G(n_1) - d_G(n_2)|}{d(n_1) + d(n_2)}]$

$$= 2 \left[\sum_{n_1n_2 \in E_{1,r+2}} + \sum_{n_1n_2 \in E_{4,r+2}} + \sum_{n_1n_2 \in E_{r+2,r+2}} \right] \left[\frac{|d_G(n_1) - d_G(n_2)|}{d(n_1) + d(n_2)} \right]$$

$$= 2 \left[(42rq + 14q - 28r - 8) \frac{|d_G(n_1) - d_G(n_2)|}{d(n_1) + d(n_2)} + (28q - 20) \frac{|d_G(n_1) - d_G(n_2)|}{d(n_1) + d(n_2)} + (21q - 14) \frac{|d_G(n_1) - d_G(n_2)|}{d(n_1) + d(n_2)} \right]$$

$$= 2[(42rq + 14q - 28r - 8) \frac{| - r - 1|}{r+3} + (28q - 20) \frac{| - r - 2|}{r+6} + (21q - 14) \left(\frac{r + 2 - r - 2}{2r+4} \right)]$$

$$= 2[(42rq + 14q - 28r - 8) \left(\frac{| - r - 1|}{r+3} \right) + (28q - 20) \left(\frac{| - r - 2|}{r+6} \right)$$

(vii) $IRGA(G) = \sum_{n_1n_2\in E(G)} ln\ \frac{d_{n_1}+d_{n_2}}{2(\sqrt{d_{n_1}d_{n_1}})} = [\sum_{n_1n_2\in E_{1,r+2}} + \sum_{n_1n_2\in E_{4,r+2}} + \sum_{n_1n_2\in E_{r+2,r+2}}]ln\ \frac{d_{n_1}+d_{n_2}}{2(\sqrt{d_{n_1}d_{n_1}})} = (42rq + 14q - 28r - 8)ln\ \frac{d_{n_1}+d_{n_2}}{2(\sqrt{d_{n_1}d_{n_1}})} + (28q - 20)ln\ \frac{d_{n_1}+d_{n_2}}{2(\sqrt{d_{n_1}d_{n_1}})} + (21q - 14)ln\ \frac{d_{n_1}+d_{n_2}}{2(\sqrt{d_{n_1}d_{n_1}})} = (42rq + 14q - 28r - 8)\left(ln\ \frac{1+r+2}{2(\sqrt{r+2})}\right) + (28q - 20)\left(ln\ \frac{4+r+2}{2(\sqrt{4(r+2)})}\right) + (21q - 14)\left(ln\ \frac{r+2+r+2}{2\left(\sqrt{(r+2)^2}\right)}\right) = (42rq + 14q - 28r - 8)\left(ln\ \frac{1+r+2}{2(\sqrt{r+2})}\right) + (28q - 20)\left(ln\ \frac{4+r+2}{2(\sqrt{4(r+2)})}\right) + (21q - 14)\left(ln\ \frac{r+2+r+2}{2\left(\sqrt{(r+2)^2}\right)}\right) = (42rq + 14q - 28r - 8)\left(ln\ \frac{r+3}{2(\sqrt{r+2})}\right) + (28q - 20)\left(ln\ \frac{r+6}{2(\sqrt{4(r+2)})}\right) + 21p - 14(ln\ (2))$

Table 4. Irregularity Indices Related to Theorem 2.

r, q	IRLU(G)	IRLU(G)	IRA(G)	IRDIF(G)	IRLF(G)	IRGA(G)	LA(G)
(1,1)	42.66	42	3.7162	16	14	7.82	26.85
(1,2)	164	161	14.22	62.67	17.89	30.72	106.85
(1,3)	285.33	280	24.72	109.34	93.34	53.61	185.85
(1,4)	406.66	399	35.2342	156	133	76.5	266.85
(1,5)	528	518	45.74	202.66	259	99.4	346.85
(1,6)	649.33	637	56.2463	249.33	212.33	122.3	426.85
(1,7)	770.66	756	66.7523	296	252	145.2	506.85
(1,8)	892	875	77.2583	342.66	191.66	168.1	586.85
(1,9)	1013.33	994	87.7643	389.33	331.33	191	666.85
(1,10)	1134.66	1113	98.27	436	371	213.9	746.85
(1,11)	1256	1232	108.7763	482.66	410.66	236.8	826.85
(1,12)	1377.33	1351	119.2824	529.33	450.33	259.7	906.85
(1,13)	1498.66	1470	129.7884	576	490	282.6	986.85
(1,14)	1620	1589	140.2944	622.66	529.66	305.5	1066.85
(1,15)	1741.33	1809	150.8	669.33	569.33	328.4	1146.85
(1,16)	1862.66	1827	161.3064	716	609	351.3	1226.85
(1,17)	1984	1946	171.8124	762.66	648.66	374.2	1306.85
(1,18)	2105.33	2065	182.3184	809.33	688.33	397.1	1386.85
(1,19)	2226.66	2184	192.8244	856	728	420	1466.85
(1,20)	2348	2303	203.33	902.66	767.66	442.9	1546.85

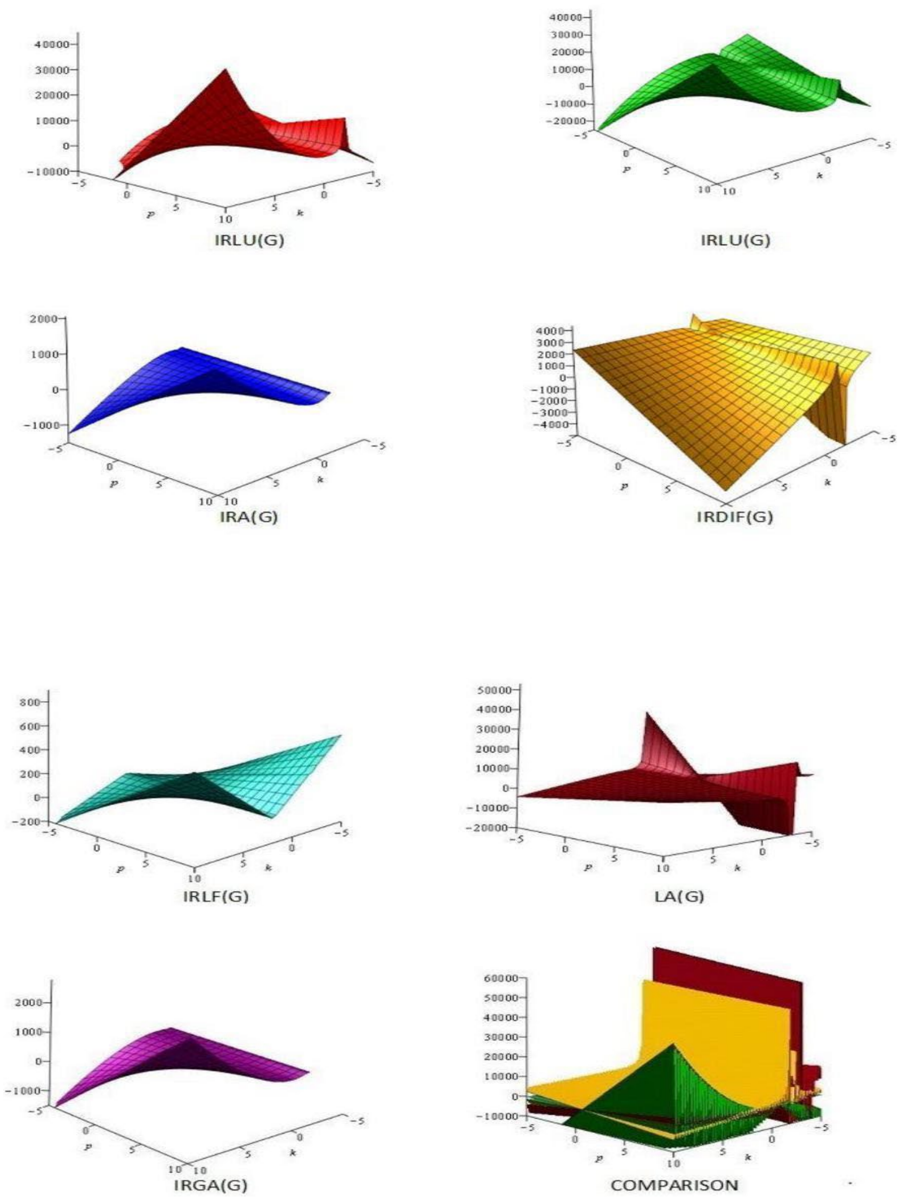


Figure 4. Comparison of the Irregularity Indices, *i.e.*, Represented by $IRLU(G), IRLU(G), IRA(G), IRDIF(G), LA(G)$, $IRGA(G), IRLF(G)$ Presented by Red, Green, Blue, Yellow, Cyan, Maroon & Purple Colors, Respectively

Among these indices $IRLU(G)$ is more dominant irregularity index for fractal-trees dendrimers.

4. IRREGULARITY INDICES FOR CAYLEY'S TREE DENDRIMERS

The Cayley tree is a type of dendrimers, which is also known as Bethe lattice Let $C_{p,q}(p \geq 3, q \geq 0)$ represents the Cayley tree dendrimers after t iterations. Initially $(q = 0), C_{p,0}$ consists of central vertex only to form $C_{p,1}$ we creates p vertices and attach them to middle vertex. For $q > 1, C_{p,q}$ is obtained from $C_{p,q-1}$ by performing $p - 1$ vertices are generated and attached to the boundary vertices.

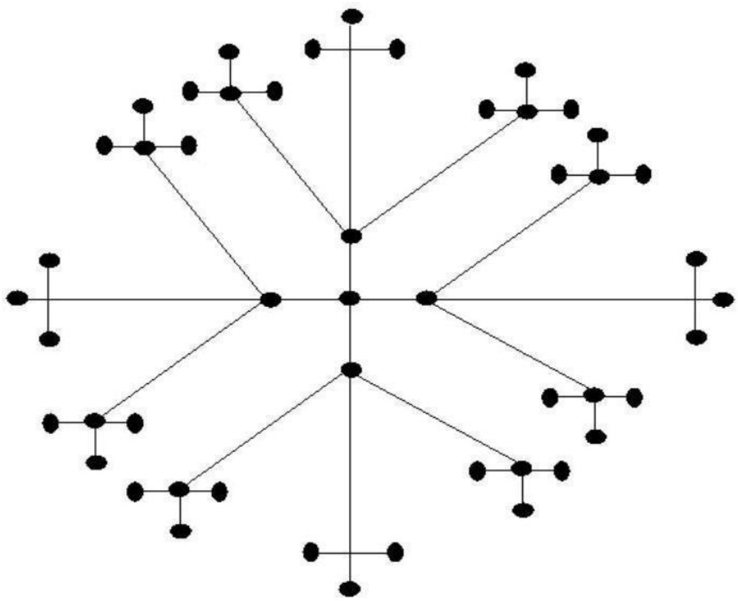


Figure 5. Cayley Tree Dendrimer $C_{4,3}$

Table 5. Sepration of Edge Set of Cayley's Tree Dendrimer Based on degrees of End Vertices

$d(n_1), d(n_1)$	$(1, r)$	(r, r)
No. of edges	$r(r-1)^{q-1}$	$r\sum_{i=1}^{q}(r-1)^{i-1} - (r(r-1)^{q-1})$

Theorem 3. Let $G \cong C_{p,q}$ be a Cayley tree dendrimer then its irregularity indices are given as

(i) $IRR(G) = (r(r-1)^{q-1})|1 - r|$.

(ii) $IRL(G) = (r(r-1)^{q-1})(ln\,(r))$.

(iii) $IRR_t(G) = \frac{1}{2}[(r(r-1)^{q-1})|1-r|]$.

(iv) $IRF(G) = (r(r-1)^{q-1})(1-r)^2$.

(v) $IRD1 = (r(r-1)^{t-1})(1-r)^2(ln\,(1+|1-r|))$.

(vi) $IRB(G) = (r(r-1)^{q-1})(1-r)^2(\sqrt{1}-\sqrt{r})^2$.

Proof:

(i) $IRRG(G) = \sum_{n_1n_2 \in E(G)} |d_G(n_1) - d_G(n_2)|$

$$= \sum_{n_1n_2 \in E_{1,p}} + \sum_{n_1n_2 \in E_{r,r}} [|d_G(n_1) - d_G(n_2)|]$$

$$= (r(r-1)^{q-1})|1-r| + r\sum_{i=1}^{q} (r-1)^{i-1}$$
$$-(r(r-1)^{q-1})|r-r| \quad = (r(r-1)^{q-1})|1-r|$$

(ii) $IRL(G) = \sum_{n_1n_2 \in E(G)} |lnd(n_1) - lnd(n_2)|$

$$= \sum_{n_1n_2 \in E_{1,s}} + \sum_{n_1n_2 \in E_{s,s}} [|lnd(n_1) - lnd(n_2)|]$$

$$= (r(r-1)^{q-1})|ln\,(1) - ln\,(r)| + r\sum_{i=1}^{t} (r-1)^{i-1}$$
$$-(r(r-1)^{t-1})|ln\,(r) - ln\,(r)|$$
$$= (r(r-1)^{t-1})(ln\,(r))$$

(iii) $IRR_t(G) = \frac{1}{2}\sum_{n_1n_2 \in E(G)} |d_G(n_1) - d_G(n_2)|$

$$= \frac{1}{2}\sum_{n_1n_2 \in E_{1,p}} + \frac{1}{2}\sum_{n_1n_2 \in E_{r,r}} [|d_G(n_1) - d_G(n_2)|]$$

$$= \frac{1}{2}\left[\begin{array}{c}(r(r-1)^{q-1})|1-r| + r\sum_{i=1}^{q} (r-1)^{i-1} \\ -(r(r-1)^{q-1})|r-r|\end{array}\right]$$

$$=\frac{1}{2}[(r(r-1)^{q-1})|1-r|]$$

(iv) $IRF(G)=\sum_{n_1n_2\in E(G)}\left(d_G(n_1)-d_G(n_2)\right)^2$

$$=\sum_{n_1n_2\in E_{1,s}}+\sum_{n_1n_2\in E_{p,p}}\left[\left(d_G(n_1)-d_G(n_2)\right)^2\right]$$

$$=(r(r-1)^{q-1})(1-r)^2+r\sum_{i=1}^{q}(r-1)^{i-1}-(r(r-1)^{q-1})(r-r)^2 \quad =(r(r-1)^{q-1})(1-r)^2$$

(v) $IRD1(G)=\sum_{n_1n_2\in E(G)}\left(ln\left(1+\left|d_{n_1}+d_{n_2}\right|\right)\right)$

$$=\sum_{n_1n_2\in E_{1,p}}+\sum_{n_1n_2\in E_{p,p}}\left[\left(ln\left(1+\left|d_{n_1}+d_{n_2}\right|\right)\right)\right]$$

$$=(r(r-1)^{q-1})(1-r)^2(ln\,(1+|1-r|))\ +r\sum_{i=1}^{q}(r-1)^{i-1}-(r(r-1)^{q-1})(ln\,(1+|r-r|))$$
$$=(r(r-1)^{q-1})(1-r)^2(ln\,(1+|1-r|))$$

(vi) $IRB(G)=\sum_{n_1n_2\in E(G)}\left(\sqrt{d_{n_1}}-\sqrt{d_{n_1}}\right)^2$

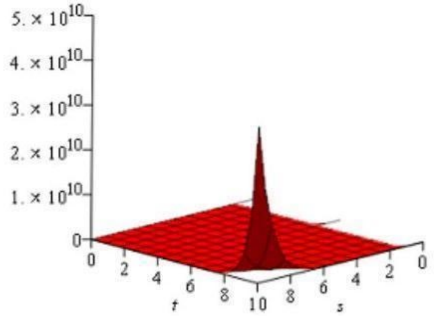
$$=\sum_{n_1n_2\in E_{1,p}}+\sum_{n_1n_2\in E_{p,p}}\left[\left(\sqrt{d_{n_1}}-\sqrt{d_(n_2)}\right)^2\right]$$

$$=(r(r-1)^{q-1})(1-r)^2(\sqrt{1}-\sqrt{r})^2+r\sum_{i=1}^{t}(r-1)^{i-1}-(r(r-1)^{t-1})(\sqrt{r}-\sqrt{r})^2$$
$$=(r(r-1)^{q-1})(1-r)^2(\sqrt{1}-\sqrt{pr}$$

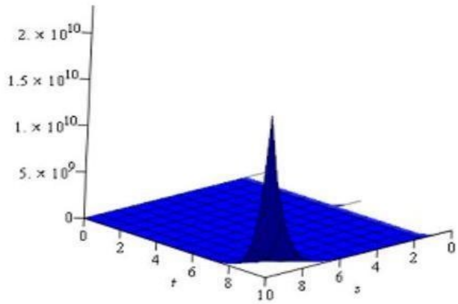
Table 6. Irregularity Indices Related to Theorem 3

p,q	IRR(G)	$IRRR_t(G)$	IRL(G)	IRF(G)	IRD1	IRB(G)
(4,1)	12	6	5.5451	36	49.9	36
(4,2)	36	18	16.6355	108	149.71	108
(4,3)	108	54	49.9	324	449.15	324

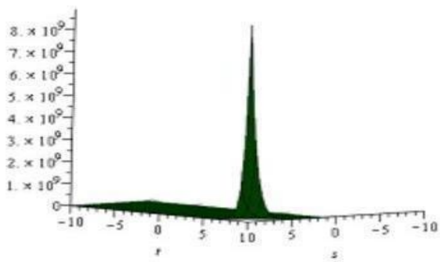
p, q	IRR(G)	$IRRR_t(G)$	IRL(G)	IRF(G)	IRD1	IRB(G)
$(4,4)$	324	162	149.71	972	1347.47	972
$(4,5)$	972	486	449.15	2916	4042.434357	2916
$(4,6)$	2916	1458	1347.47	8748	12127.30307	8748
$(4,7)$	8748	4374	4042.42	26244	36381.90921	26244
$(4,8)$	26244	13122	12127.3	78732	109145.7276	78732
$(4,9)$	78732	39366	36381.9	236196	327437.1829	236196
$(4,10)$	236196	118098	109145.72	708588	982311.5488	708588
$(4,11)$	708588	354294	327437.18	2125764	2646934.646	2125764
$(4,12)$	21225764	1062882	982311.54	6377292	8840803.939	6377292
$(4,13)$	6377292	3186146	2946934064	19131876	26522411.82	19131876
$(4,14)$	19131876	95655938	8840803.93	573956228	79567235.45	573956228
$(4,15)$	57395628	28697814	79567235.45	172186884	2387017063	172186884
$(4,16)$	172186884	86093442	26522411.82	516560652	716105119	516560652
$(4,17)$	515160652	258280326	238701706	1549681956	2148315357	1549681956



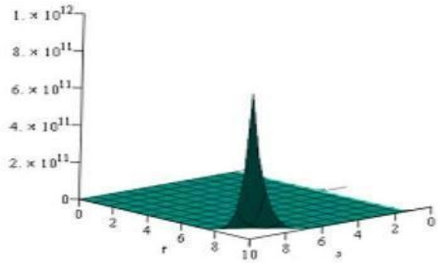
$irr(G)$



$IRR_t(G)$



$IRL(G)$



$IRF(G)$

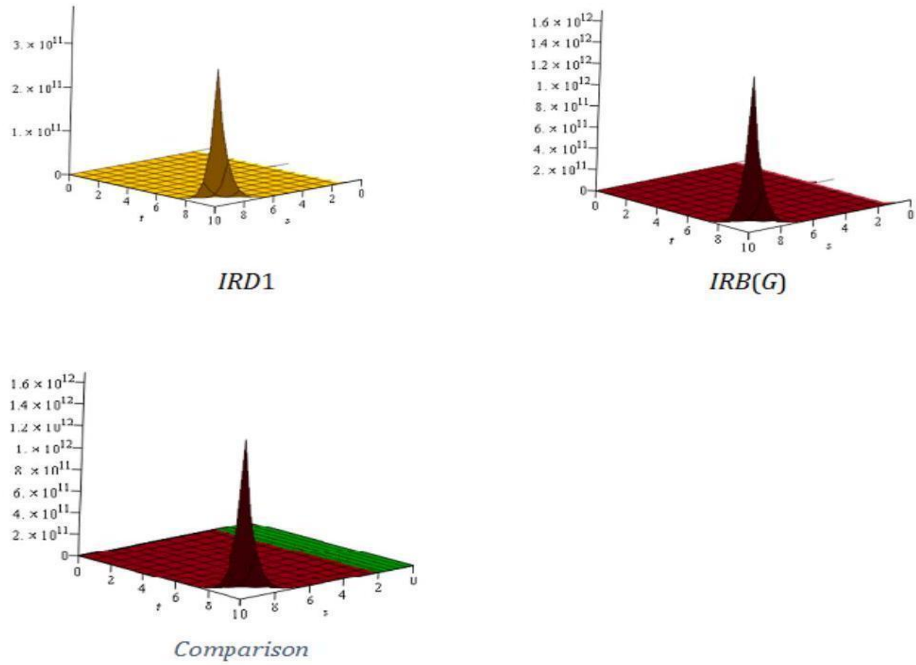


Figure 6. Comparison of the Irregularity Indices, *i.e.*, $IRR(G), IRR_t(G), IRL(G), IRF(G), IRD1(G), IRB(G)$ are Indicated as Red, Green, Blue, Teal, Yellow and Plum Colours Respectively.

Among these indices $IRD1(G)$ is more dominant irregularity index for Cayley tree dendrimers.

Theorem 4. Let $G \cong C_{p,q}$ be a Cayley tree dendrimer then its irregularity indices are given as

(i) $IRLU(G) = (r(r-1)^{q-1})|(1-r)|$.

(ii) $IRA(G) = (r(r-1)^{q-1})(1-r)^2 \frac{(\sqrt{r}-1)^2}{r}$.

(iii) $IRDIE(G) = (r(r-1)^{q-1})(1-r)^2 \left(\left|\frac{1-r}{r}\right|\right)$.

(iv) $IRLF(G) = (r(r-1)^{q-1})(1-r)^2 \frac{|1-r|}{r}$.

(v) $LA(G) = 2\left[(r(r-1)^{q-1})(1-r)^2 \frac{|1-r|}{r+1}\right]$.

(vi) $IRGA(G) = (r(r-1)^{q-1})(1-r)^2 \left(ln\ \frac{1+r}{2(\sqrt{r})}\right)$.

Proof.:

(i) $IRLU(G) = \frac{\sum_{n_1 n_2 \in E_{1,p}} |d(n_1) - d(n_2)|}{min(d(n_1), d(n_2))}$

$$= \left[\sum_{n_1 n_2 \in E_{1,p}} + \sum_{n_1 n_2 \in E_{p,p}} \right] \frac{|d(n_1) - d(n_2)|}{min(d(n_1), d(n_2))}$$

$$= (s(s-1)^{t-1}) \frac{|1-r|}{1} = (r(r-1)^{q-1})(1-r)$$

(ii) $IRA(G) = \sum_{n_1 n_2 \in E(G)} \left(\frac{1}{\sqrt{d(n_1)}} - \frac{1}{\sqrt{d(n_2)}} \right)^2$

$$= \left[\sum_{n_1 n_2 \in E_{1,p}} + \sum_{n_1 n_2 \in E_{p,p}} \right] \left(\frac{1}{\sqrt{d(n_1)}} - \frac{1}{\sqrt{d(n_2)}} \right)^2$$

$$= (r(r-1)^{q-1})(1-r)^2 \left(\frac{1}{\sqrt{1}} - \frac{1}{\sqrt{r}} \right)^2$$

$$= (r(r-1)^{q-1})(1-r)^2 \frac{(\sqrt{r}-1)^2}{r}$$

(iii) $IRDIE(G) = \sum_{n_1 n_2 \in E(G)} \left(\left| \frac{d(n_1)}{d(n_2)} - \frac{d(n_2)}{d(n_2)} \right| \right)$

$$= \left[\sum_{n_1 n_2 \in E_{1,p}} + \sum_{n_1 n_2 \in E_{p,p}} \right] \left(\left| \frac{d(n_1)}{d(n_2)} - \frac{d(n_2)}{d(n_2)} \right| \right)$$

$$= (r(r-1)^{q-1})(1-r)^2 \left(\left| \frac{1}{r} - \frac{r}{r} \right| \right)$$

$$= (r(r-1)^{t-1})(1-r)^2 \left(\left| \frac{1-r}{r} \right| \right)$$

(iv) $IRLF(G) = \sum_{n_1 n_2 \in E(G)} \frac{|d_G(n_1)) - d_G(n_2))|}{d(n_2))d(n_1))}$

$$= \left[\sum_{n_1 n_2 \in E_{1,s}} + \sum_{n_1 n_2 \in E_{s,s}} \right] \frac{|\, d_G(n_1)) - d_G(n_2))\, |}{d(n_2))d(n_1))}$$

$$= (r(r-1)^{q-1})(1-r)^2 \frac{|1-r|}{r} = (r(r-1)^{q-1})(1-r)^2 \frac{|1-r|}{r}$$

(v) $LA(G) = 2\sum_{n_1n_2\in E(G)} \frac{|d_G(n_1)) - d_G(n_2))|}{d(n_1)) + d(n_2))}$

$$= \left[\sum_{n_1n_2\in E_{1,s}} + \sum_{n_1n_2\in E_{s,s}}\right] \frac{|\ d_G(n_1)) - d_G(n_2))\ |}{d(n_1)) + d(n_2))}$$

$$= 2\left[(r(r-1)^{q-1})(1-r)^2 \frac{|1-r|}{r+1}\right]$$

$$= 2\left[(r(r-1)^{q-1})(1-r)^2 \frac{|1-r|}{r+1}\right]$$

(vi) $IRGA(G) = \sum_{n_1n_2\in E(G)} ln\ \frac{d_{n_1} + d_{n_1}}{2(\sqrt{d_{n_1}d_{n_1}})}$

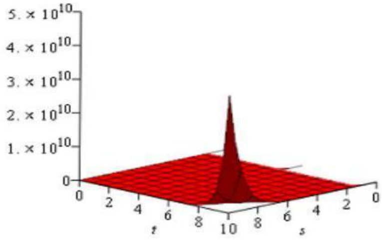
$$= \left[\sum_{n_1n_2\in E_{1,p}} + \sum_{n_1n_2\in E_{p,p}}\right] ln\ \frac{d_{n_1} + d_{n_1}}{2(\sqrt{d_{n_1}d_{n_1}})}$$

$$= (r(r-1)^{q-1})(1-r)^2 \left(ln\ \frac{1+r}{2(r)}\right)$$

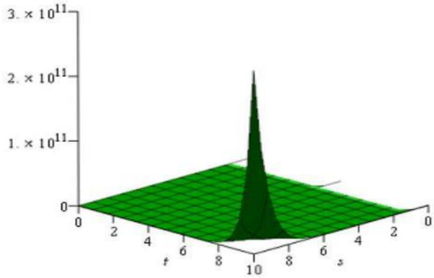
$$= (r(r-1)^{q-1})(1-r)^2 \left(ln\ \frac{1+r}{2(\sqrt{r})}\right)$$

Table 7. Irregularity Indices Related to Theorem 4

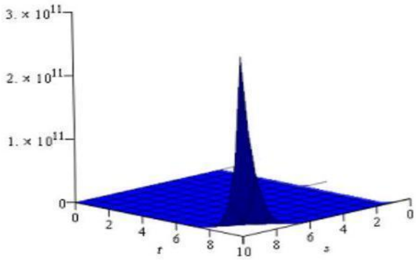
p, q	IRLU(G)	IRA(G)	IRDIF(G)	LA(G)	IRLF(G)	IRGA(G)
(4,1)	12	9	27	43.2	27	8.0331
(4,2)	36	27	81	129.6	81	24.0995
(4,3)	108	81	243	288.8	243	72.2985
(4,4)	324	243	729	1166.4	729	216.8955
(4,5)	972	729	2187	3499.2	2187	650.6865
(4,6)	2916	2187	6561	10497.6	6561	1952.059
(4,7)	8748	6561	19683	31492.8	19683	5856.173
(4,8)	26244	19683	59049	94478.4	59049	17568.538
(4,9)	78732	59049	177147	283435.2	177147	52705.6142
(4,10)	236196	177147	531441	850305.6	531441	158116.8424
(4,11)	708588	531441	1594323	2550916.8	1594323	1423051.585
(4,12)	2125764	1594323	4782969	7652750.4	4782969	4269154.754
(4,13)	6377292	4782969	14348907	22958251.2	14348907	12807464.26
(4,14)	19131876	14348907	43046721	68874753.6	43046721	38422392.29
(4,15)	57395628	43046721	129140162	206624260.8	129140162	115267178.4
(4,16)	172186884	129140162	387420489	619872782.4	387420489	345801535.1
(4,17)	515160652	387420489	387420489	1859618347	387420489	1037404605



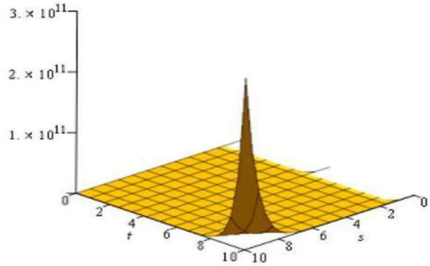
$IRLU(G)$



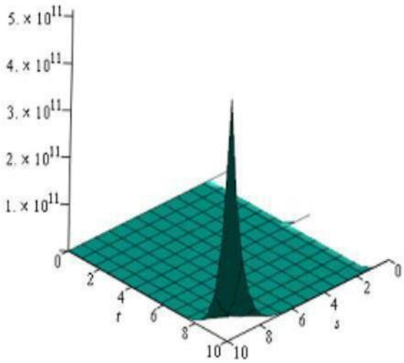
$IRA(G)$



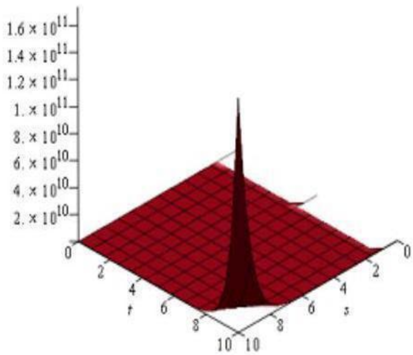
$IRDIE(G)$



$IRLF\,(G)$



$LA(G)$



$IRGA(G)$

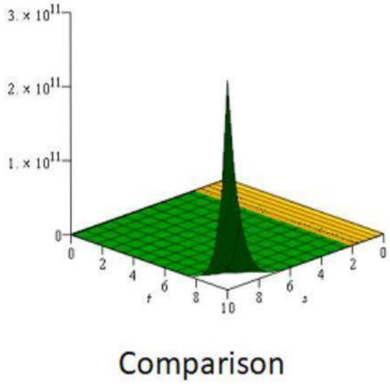


Figure 7. Comparison of the Irregularity Indices, *i.e.*, $IRLU(G), IRDIF(G), IRA(G), LA(G), IRLF(G), IRGA(G)$ are indicated as Red, Green, Blue, Yellow, Cyan and Maroon Colours

Among these indices $LA(G)$ is a more dominant irregularity index for Cayley tree dendrimers.

5. CONCLUSION

Dendrimers grow in patterns similar to trees or fractals found in nature. This repeating, organized structure allows scientists to control their shape very precisely. As a result, these molecules are very useful for targeted drug delivery, designing new nanomaterials, and speeding up chemical reactions. Their branching architecture also makes them efficient, flexible, and easy to adapt for advanced chemical and biomedical applications. In conclusion, various irregularity indices for fractal- and Cayley-tree dendrimers are determined. The results are presented through tables containing numerical values and figures showcasing graphical representations. Our analysis revealed that IRD1 is the most dominant and consistent index among the fractal- and Cayley-tree dendrimers.

CONFLICT OF INTEREST

The authors of the manuscript have no financial or non-financial conflict of interest in the subject matter or materials discussed in this manuscript.

DATA AVAILABILITY STATEMENT

The data is freely-available and the reference paper is cited in data analysis section.

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