

# Topological Properties of Subdivided Hex-derived Networks

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Received: 20 November 2022; Accepted: 12 December 2022; Published: 30 December 2022.

**Abstract:** A non-empirical numerical value that grasp properties of molecular graph of chemical structure referred to as topological index. Topological indices of molecular graph are very useful for scientist to accomplish regression analysis in QSPR study. In this paper, we will use latest technique (Imbalanced based indices) to associate a numeric quantity with a the molecular graph of Subdivided Hex-derived networks  $SHN_t$ .

**Keywords:** Irregularity indices, Subdivided Hex-derived networks.

## 1. Introduction and Preliminaries

The construction of  $SHN_t$  is simple. We can construct  $SHN_t$  by the subdivision of hexderived by adding extra points in every triangle the hexagonal mesh's face and then attach this extra point with all other existing points. In [1], one can find out an alternative construction of  $SHN_t$ . The comparison of  $HN_t$  and  $SHN_t$  shows that this new  $SHN_t$  derived network have some new and exiting properties. It presents the configuration like wise molecular lattice shapes in chemistry. Moreover  $SHN_t$  is a mesh network [2], mesh networks play an important rule in networking, where cost minimize problems exit.

In mathematical chemistry, graph theory offers the trusty tool that is used to compute the numerous types of chemical compounds and anticipate their various attributes. A topological index (TI), which is effective in predicting the chemical and physical properties of the underlying chemical compound, such as boiling point, strain energy, stiffness, heat of evaporation, tension, and so on, is one of the most crucial tools in chemical graph theory. [3,4]. A simple graph is one without several loops or edges. A molecular graph is a simple graph with the vertex and edge sets represent, respectively, atoms and bounds. The amount of edges that are connected to a vertex determines its degree. It is mostly interesting these characteristics of diverse. Winner discovered the boiling point in 1947 and introduced the first. In 1975, Gutman provided an impressive identity [5] about Zagreb indices. As a result, these two indices are some of the first degree-based descriptors, and substantial research has been done on their characteristics. These indices' mathematical formulas are:  $G$

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v),$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v).$$

For various chemical architectures and networks, many authors calculated TIs, such as in [6], Amin et al. studied prism graphs. For the prism graph, they calculated M-polynomial and nine-degree based indices. TIs of Circulate graphs has been studied by Gao et al. in [7]. Dobrynin et al. in [8] talk about the wiener index for tree graphs. Researchers have looked into the idea of mathematical chemistry and its characteristics in [9]. Caporossi at al. in [10], describe the highest connection index for several graphs. Li and Gutman, With chemical graph theory, discuss the chemical composition of monographs [11]. Li and Shi in [12], gives a details analysis of famous Randić index. The survey on Zagreb indices was put forward by Nikolić et al. in [13]. Another survey on Zagreb indices was written by Gutman and Das in [14]. Virk et al. in [15], changed the Atomic Bond Connectivity Index definition that was previously provided and provided a new definition.

Shao et al. [16] gives topological characteristics of Bismuth Tri-Iodide. In [17], Virk et al. discuss the reverse Zagreb indices for Silicon Carbides.

A TI is recognized as Irregularity index, [18] if the value of TI of graph is higher or equal to zero and TI of graph will be zero if graph have homogenous degree of nodes throughout the graph. The Irregularity indices are listed below. The majority of irregularity indices used in quantitative structure activity relationship modelling come from the family of degree-based TIs. Mathematical definition of irregularity indices are in table 1,

**Table 1.** Definitions of Irregularity indices

Irregularity index	Mathematical Formula
VAR	$\sum_{u \in V} (d_u - \frac{2m}{n})^2 = \frac{M_1(\mathbb{G})}{n} - (\frac{2m}{n})^2$
AL	$\sum_{uv \in E(\mathbb{G})}  d_u - d_v $
IR1	$\sum_{u \in V} (d_u)^3 - \frac{2m}{n} \sum_{u \in V} (d_u)^2 = F(\mathbb{G}) - \frac{2m}{n} M_1(\mathbb{G})$
IR2	$\sqrt{\frac{\sum_{uv \in E(\mathbb{G})} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(\mathbb{G})}{m}} - \frac{2m}{n}$
IRF	$\sum_{uv \in E(\mathbb{G})} (d_u - d_v)^2 = F(\mathbb{G}) - 2M_2(\mathbb{G})$
IRFW	$\frac{IRF(\mathbb{G})}{M_2(\mathbb{G})}$
IRA	$\sum_{uv \in E(\mathbb{G})} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(\mathbb{G})$
IRB	$\sum_{uv \in E(\mathbb{G})} (d_u^{1/2} - d_v^{1/2})^2 = M_1(\mathbb{G}) - 2RR(\mathbb{G})$
IRC	$\frac{\sum_{uv \in E(\mathbb{G})} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(\mathbb{G})}{m} - \frac{2m}{n}$
IRDIF	$\sum_{uv \in E(\mathbb{G})} \left  \frac{d_u}{d_v} - \frac{d_v}{d_u} \right  = \sum_{i < j} m_{i,j} \left( \frac{i}{j} - \frac{j}{i} \right)$
IRL	$\sum_{uv \in E(\mathbb{G})}  \ln d_u - \ln d_v  = \sum_{i < j} m_{i,j} \ln \left( \frac{i}{j} \right)$
IRLU	$\sum_{uv \in E(\mathbb{G})} \frac{ d_u - d_v }{\min(d_u, d_v)} = \sum_{i < j} m_{i,j} \ln \left( \frac{i-j}{i} \right)$
IRLF	$\sum_{uv \in E(\mathbb{G})} \frac{ d_u - d_v }{\sqrt{(d_u d_v)}} = \sum_{i < j} m_{i,j} \left( \frac{i-j}{\sqrt{ij}} \right)$
IRLA	$2 \sum_{uv \in E(\mathbb{G})} \frac{ d_u - d_v }{(d_u + d_v)} = 2 \sum_{i < j} m_{i,j} \left( \frac{i-j}{i+j} \right)$
IRDI	$\sum_{uv \in E(\mathbb{G})} \ln 1 +  d_u - d_v  = \sum_{i < j} m_{i,j} \ln(i + j - 1)$
IRGA	$\sum_{uv \in E(\mathbb{G})} \ln \left( \frac{d_u + d_v}{2\sqrt{d_u d_v}} \right) = \sum_{i < j} m_{i,j} \ln \left( \frac{i+j}{2\sqrt{ij}} \right)$

## 2. Irregularity indices for Subdivided Hex-derived networks $SHN_t$

The network under consideration  $SHN_t$ , obtain by carry out the subdivision of hex-derived network  $HN_t$ . Here, we'll talk about the erratic character of  $SHN_t$  graph with the help of irregularity indices. The 2D graph of  $SHN_t$  is given in Figure 2. From figure 2, we can see, that  $SHN_p$  graph have four different types of edges depending upon the degree of end vertices. Such that,  $E(SHN_t) = \mathcal{P}_1 + \mathcal{P}_2 + \mathcal{P}_3 + \mathcal{P}_4$  and the cardinality of  $|E(SHN_p)| = 27t^2 - 51t + 24$  The extra knowledge for various edges of  $SHN_t$  is illustrated in Table 2.

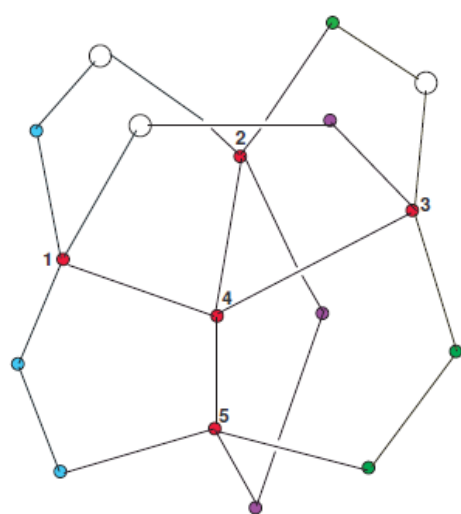


Figure 1. Subdivision of  $K - 5$  inside Simmons-Paquette molecular graph

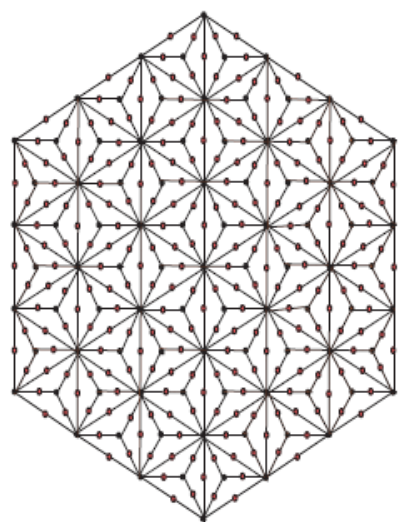


Figure 2. graph of  $SHN_t$

Table 2.  $E(SHN_t)$

Edge Division	Edge Splitting	Reoccurrence
$\mathcal{P}_1$	$\mathcal{P}_{(2,3)}$	$18t^2 - 36t + 18$
$\mathcal{P}_2$	$\mathcal{P}_{(2,5)}$	30
$\mathcal{P}_3$	$\mathcal{P}_{(2,7)}$	$42t - 84$
$\mathcal{P}_4$	$\mathcal{P}_{(2,12)}$	$36t^2 - 108t + 84$

**Theorem 1.** Let  $\mathbb{G}$  be the graph of  $SHN_t$ . The Irregularity indices are

1.  $VAR(\mathbb{G}) = -\frac{2(1035t^4 + 1110t^3 - 5630t^2 + 5103t - 1368)}{(9t^2 - 15t + 7)^2}$
2.  $AL(\mathbb{G}) = 378t^2 - 906t + 528$
3.  $IR1(\mathbb{G}) = \frac{6(3285t^4 + 102344t^3 - 361514t^2 + 401189t - 143254)}{9t^2 - 15t + 7}$

$$\begin{aligned}
4. \text{IR2}(\mathbb{G}) &= \sqrt{\frac{972t^2 - 2220t + 1248}{27t^2 - 51t + 24}} - \frac{2(27t^2 - 51t + 24)}{9t^2 - 15t + 7} \\
5. \text{IRF}(\mathbb{G}) &= 3618t^2 - 9786t + 6588 \\
6. \text{IRFW}(\mathbb{G}) &= \frac{3618t^2 - 9786t + 6588}{972t^2 - 2220t + 1248}
\end{aligned}$$

**Proof.**

$$\begin{aligned}
\text{VAR}(\mathbb{G}) &= \sum_{u \in V} \left( d_u - \frac{2m}{n} \right)^2 = \frac{M_1(\mathbb{G})}{n} - \left( \frac{2m}{n} \right)^2 \\
&= \left( \frac{(94t^2 - 1314t + 720)}{9t^2 - 15t + 7} \right) - \left( \frac{2(27t^2 - 51t + 24)}{(9t^2 - 15t + 7)} \right)^2 \\
&= -\frac{2(1035t^4 + 1110t^3 - 5630t^2 + 5103t - 1368)}{(9t^2 - 15t + 7)^2}.
\end{aligned}$$

$$\begin{aligned}
\text{AL}(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} |d_u - d_v| \\
&= |2 - 3|(18t^2 - 36t + 18) + |2 - 5|(30) + |2 - 7|(42t - 84) \\
&\quad + |2 - 12|(36t^2 - 108t + 84) \\
&= 378t^2 - 906t + 528.
\end{aligned}$$

$$\begin{aligned}
\text{IR1}(\mathbb{G}) &= \sum_{u \in V} d_u^3 - \frac{2m}{n} \sum_{u \in V} d_u^2 = F(\mathbb{G}) - \left( \frac{2m}{n} \right) M_1(\mathbb{G}) \\
&= (5562t^2 - 14226t + 20964) - \left( \frac{2(27t^2 - 51t + 24)}{9t^2 - 15t + 7} \right) \\
&\quad (562t^2 - 14226t + 20964) \\
&= \frac{6(3285t^4 + 102344t^3 - 361514t^2 + 401189t - 143254)}{9t^2 - 15t + 7}.
\end{aligned}$$

$$\begin{aligned}
\text{IR2}(\mathbb{G}) &= \sqrt{\frac{\sum_{uv \in E(\mathbb{G})} d_u d_v}{m}} - \frac{2m}{n} = \sqrt{\frac{M_2(\mathbb{G})}{m}} - \frac{2m}{n} \\
&= \sqrt{\frac{972t^2 - 2220t + 1248}{27t^2 - 51t + 24}} - \frac{2(27t^2 - 51t + 24)}{9t^2 - 15t + 7}.
\end{aligned}$$

$$\begin{aligned}
\text{IRF}(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} (d_u - d_v)^2 \\
&= (2 - 3)^2(18t^2 - 36t + 18) + (2 - 5)^2(30) + (2 - 7)^2(42t - 84) \\
&\quad + (2 - 12)^2(36t^2 - 108t + 84) \\
&= 3618t^2 - 9786t + 6588.
\end{aligned}$$

$$\begin{aligned}
\text{IRFW}(\mathbb{G}) &= \frac{\text{IRF}(\mathbb{G})}{M_2(\mathbb{G})} \\
&= \frac{3618t^2 - 9786t + 6588}{972t^2 - 2220t + 1248}.
\end{aligned}$$

□

**Theorem 2.** Let  $\mathbb{G}$  be the graph of  $\text{SHN}_t$ . The Irregularity indices are

1.  $\text{IRA}(\mathbb{G}) = 9t^2 - 15t + 7 - 12\sqrt{6}t^2 + 30\sqrt{6}t - 6\sqrt{14}t - 20\sqrt{6} - 6\sqrt{10} + 12\sqrt{14}$ .
2.  $\text{IRB}(\mathbb{G}) = 594t^2 - 1314t + 720 - 180\sqrt{6}t^2 + 504\sqrt{6}t - 84\sqrt{14}t - 372\sqrt{6} - 60\sqrt{10} + 168\sqrt{14}$ .

$$3. \text{IRC}(\mathbb{G}) = \frac{1}{3(9t^2-17t+8)(9t^2-15t+7)} (54\sqrt{6}t^4 - 225\sqrt{6}t^3 + 27\sqrt{14}t^3 + 357\sqrt{6}t^2 - 99\sqrt{14}t^2 + 27\sqrt{10}t^2 - 1458t^4 - 255\sqrt{6}t + 111\sqrt{14}t - 45\sqrt{10}t + 5508t^3 + 70\sqrt{6} - 42\sqrt{14} + 21\sqrt{10} - 7794t^2 + 4896t - 1152).$$

**Proof.**

$$\begin{aligned} \text{IRA}(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} (d_u^{-1/2} - d_v^{-1/2})^2 = n - 2R(\mathbb{G}) \\ &= (9t^2 - 15t + 7) - 2(6\sqrt{6}t^2 - 15\sqrt{6}t + 3\sqrt{14}t + 10\sqrt{6} + 3\sqrt{10} - 6\sqrt{14}) \\ &= 9t^2 - 15t + 7 - 12\sqrt{6}t^2 + 30\sqrt{6}t - 6\sqrt{14}t - 20\sqrt{6} - 6\sqrt{10} + 12\sqrt{14}. \end{aligned}$$

$$\begin{aligned} \text{IRB}(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} (d_u^{1/2} - d_v^{1/2})^2 = M_1(\mathbb{G}) - 2RR(\mathbb{G}) \\ &= (59t^2 - 1314t + 720) - 2(90\sqrt{6}t^2 - 252\sqrt{6}t + 42\sqrt{14}t + 186\sqrt{6} + 30\sqrt{10} - 84\sqrt{14}) \\ &= 594t^2 - 1314t + 720 - 180\sqrt{6}t^2 + 504\sqrt{6}t - 84\sqrt{14}t - 372\sqrt{6} - 60\sqrt{10} + 168\sqrt{14}. \end{aligned}$$

$$\begin{aligned} \text{IRC}(\mathbb{G}) &= \frac{\sum_{uv \in E(\mathbb{G})} \sqrt{d_u d_v}}{m} - \frac{2m}{n} = \frac{RR(\mathbb{G})}{m} - \frac{2m}{n} \\ &= \left( \frac{6\sqrt{6}t^2 - 15\sqrt{6}t + 3\sqrt{14}t + 10\sqrt{6} + 3\sqrt{10} - 6\sqrt{14}}{27t^2 - 51t + 24} \right) \\ &\quad - \left( \frac{2(2t^2 - 51t + 24)}{9t^2 - 15t + 7} \right) \\ &= \frac{1}{3(9t^2 - 17t + 8)(9t^2 - 15t + 7)} (54\sqrt{6}t^4 - 225\sqrt{6}t^3 + 27\sqrt{14}t^3 \\ &\quad + 357\sqrt{6}t^2 - 99\sqrt{14}t^2 + 27\sqrt{10}t^2 - 1458t^4 - 255\sqrt{6}t + 111\sqrt{14}t - 45\sqrt{10}t \\ &\quad + 5508t^3 + 70\sqrt{6} - 42\sqrt{14} + 21\sqrt{10} - 7794t^2 + 4896t - 1152). \end{aligned}$$

□

**Theorem 3.** Let  $\mathbb{G}$  be the graph of  $SHN_t$ . The Irregularity indices are

1.  $\text{IRDIF}(\mathbb{G}) = 224.92t^2 - 525.02t + 298.27.$
2.  $\text{IRL}(\mathbb{G}) = 71.64t^2 - 155.22t + 79.86.$
3.  $\text{IRLU}(\mathbb{G}) = 189t^2 - 453t + 264.$
4.  $\text{IRLF}(\mathbb{G}) = 80.64t^2 - 178.86t + 95.04.$
5.  $\text{IRLA}(\mathbb{G}) = 58.32t^2 - 121.14t + 58.74.$
6.  $\text{IRD1}(\mathbb{G}) = 98.46t^2 - 207.78t + 104.22.$
7.  $\text{IRGA}(\mathbb{G}) = 16.20t^2 - 37.44t + 20.88.$

**Proof.**

$$\begin{aligned} \text{IRDIF}(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} \left| \frac{d_u}{d_v} - \frac{d_v}{d_u} \right| \\ &= \left| \frac{2}{3} - \frac{3}{2} \right| (18t^2 - 36t + 18) + \left| \frac{2}{5} - \frac{5}{2} \right| (30) + \left| \frac{2}{7} - \frac{7}{2} \right| (42t - 84) \\ &\quad + \left| \frac{2}{12} - \frac{12}{2} \right| (36t^2 - 108t + 84) \\ &= 224.92t^2 - 525.02t + 298.27. \end{aligned}$$

$$\begin{aligned}
IRL(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} |lnd_u - lnd_v| \\
&= |ln2 - ln3|(18t^2 - 36t + 18) + |ln2 - ln5|(30) + |ln2 - ln7|(42t - 84) \\
&\quad + |ln2 - ln12|(36t^2 - 108t + 84) \\
&= 71.64t^2 - 155.22t + 79.86.
\end{aligned}$$

$$\begin{aligned}
IRLU(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} \frac{|d_u - d_v|}{\min(d_u, d_v)} \\
&= \frac{|2-3|}{2}(18t^2 - 36t + 18) + \frac{|2-5|}{2}(30) + \frac{|2-7|}{2}(42t - 84) \\
&\quad + \frac{|2-12|}{2}(36t^2 - 108t + 84) \\
&= 189t^2 - 453t + 264.
\end{aligned}$$

$$\begin{aligned}
IRLF(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} \frac{|d_u - d_v|}{\sqrt{d_u \cdot d_v}} \\
&= \frac{|2-3|}{\sqrt{6}}(18t^2 - 36t + 18) + \frac{|2-5|}{\sqrt{10}}(30) + \frac{|2-7|}{\sqrt{14}}(42t - 84) \\
&\quad + \frac{|6-8|}{\sqrt{48}}(36t^2 - 108t + 84) \\
&= 80.64t^2 - 178.86t + 95.04.
\end{aligned}$$

$$\begin{aligned}
IRLA(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} 2 \frac{|d_u - d_v|}{(d_u + d_v)} \\
&= 2 \frac{|2-3|}{5}(18t^2 - 36t + 18) + 2 \frac{|2-5|}{7}(30) + 2 \frac{|2-7|}{9}(42t - 84) \\
&\quad + 2 \frac{|2-12|}{14}(36t^2 - 108t + 84) \\
&= 58.32t^2 - 121.14t + 58.74.
\end{aligned}$$

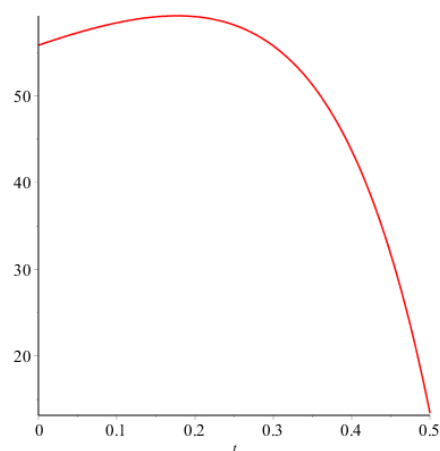
$$\begin{aligned}
IRD1(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} \ln\{1 + |d_u - d_v|\} \\
&= \ln\{1 + |2-3|\}(18t^2 - 36t + 18) + \ln\{1 + |2-5|\}(30) + \ln\{1 + |2-7|\}(42t - 84) \\
&\quad + \ln\{1 + |2-12|\}(36t^2 - 108t + 84) \\
&= 98.46t^2 - 207.78t + 104.22.
\end{aligned}$$

$$\begin{aligned}
IRGA(\mathbb{G}) &= \sum_{uv \in E(\mathbb{G})} \ln\left(\frac{d_u + d_v}{2\sqrt{d_u d_v}}\right) \\
&= \ln\left(\frac{2+3}{2\sqrt{2 \times 3}}\right)(18t^2 - 36t + 18) + \ln\left(\frac{2+5}{2\sqrt{2 \times 5}}\right)(30) + \ln\left(\frac{2+7}{2\sqrt{2 \times 7}}\right)(42t - 84) \\
&\quad + \ln\left(\frac{2+12}{2\sqrt{2 \times 12}}\right)(36t^2 - 108t + 84) \\
&= 16.20t^2 - 37.44t + 20.88.
\end{aligned}$$

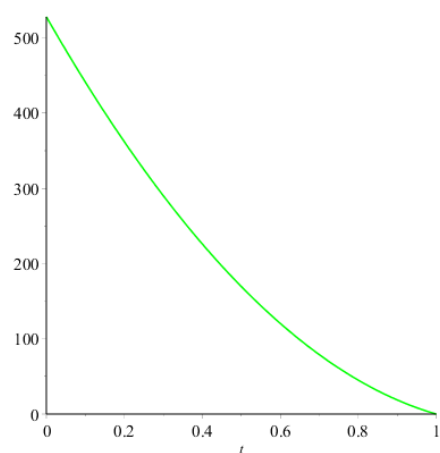
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### 3. Graphical Representation and discussion of results

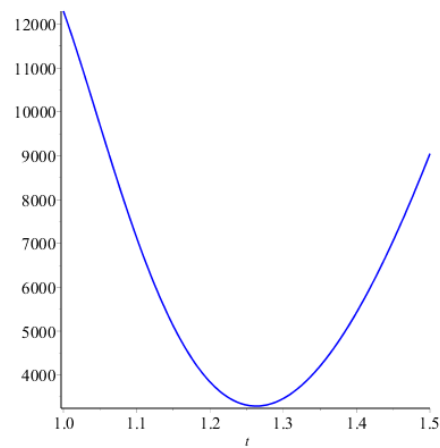
This section is about the graphical representation of  $SHN_t$ . We plot our results of sixteen irregularity indices for  $SHN_t$ .



**Figure 3.** Dendrimer Architecture



**Figure 4.** Dendrimer Architecture



**Figure 5.** Dendrimer Architecture

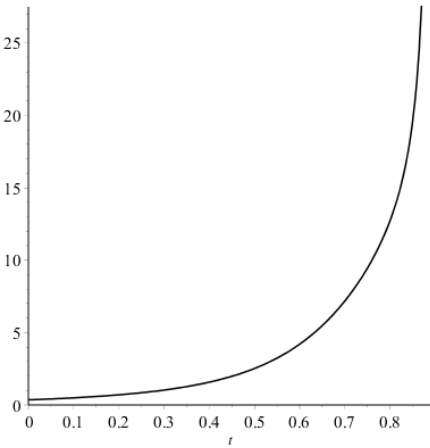


Figure 6. Dendrimer Architecture

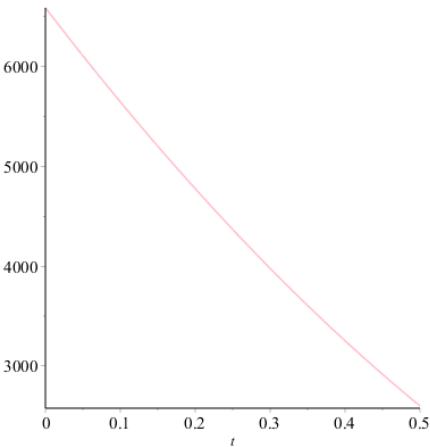


Figure 7. Dendrimer Architecture

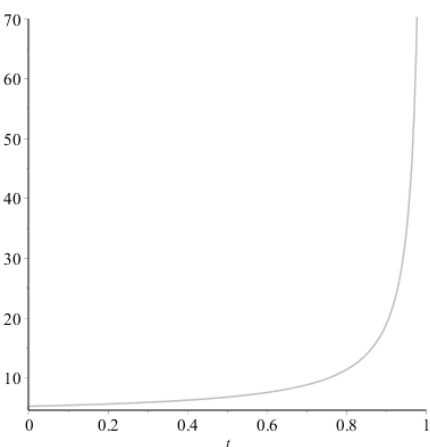


Figure 8. Dendrimer Architecture



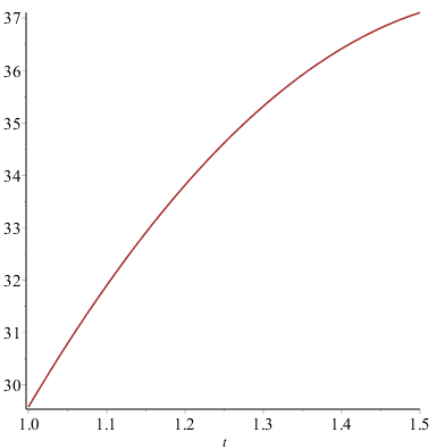


Figure 9. Dendrimer Architecture

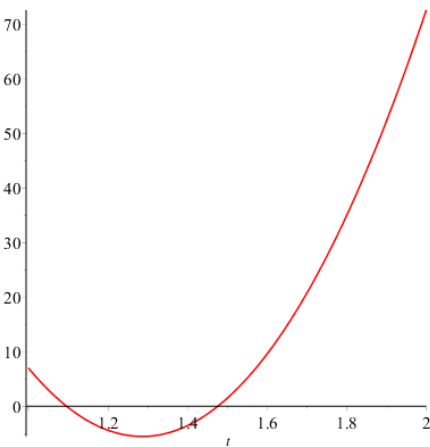


Figure 10. Dendrimer Architecture

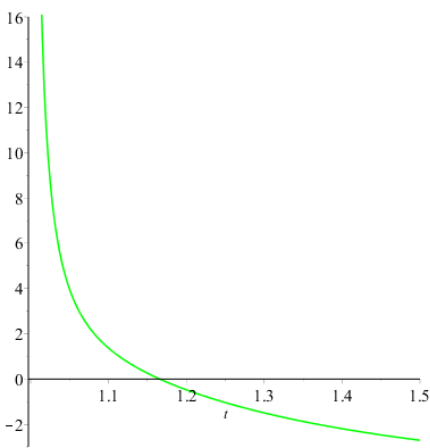


Figure 11. Dendrimer Architecture

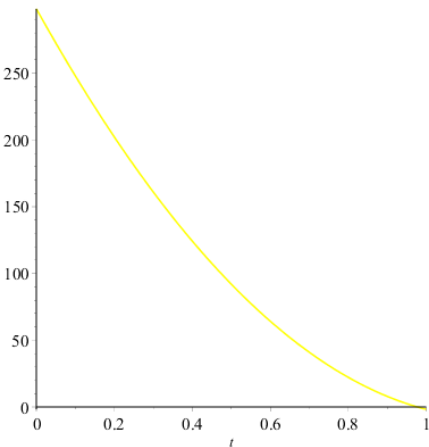


Figure 12. Dendrimer Architecture

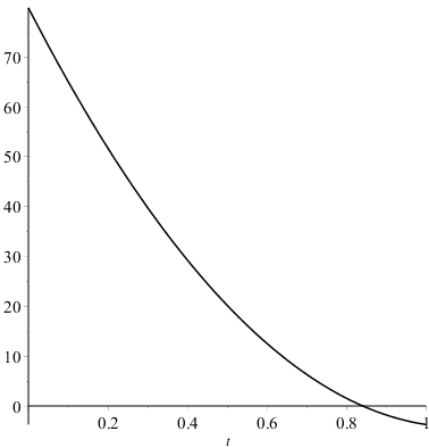


Figure 13. Dendrimer Architecture

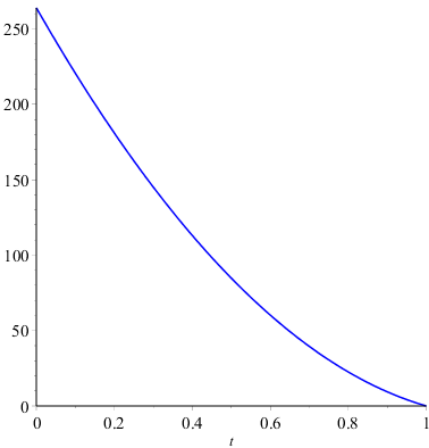


Figure 14. Dendrimer Architecture

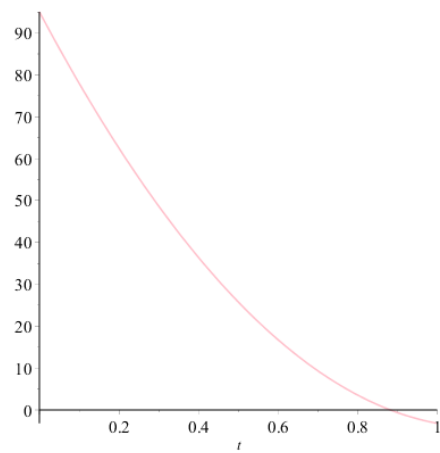


Figure 15. Dendrimer Architecture

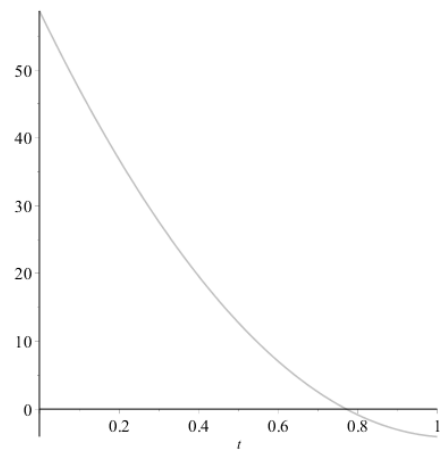


Figure 16. Dendrimer Architecture

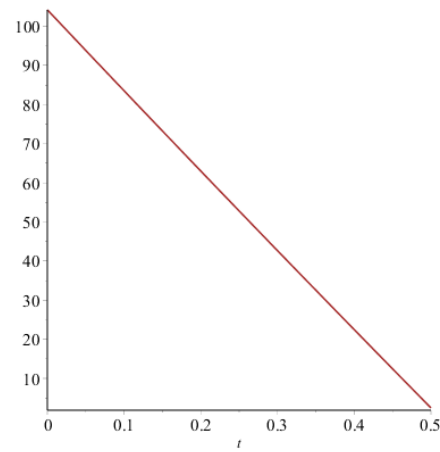


Figure 17. Dendrimer Architecture

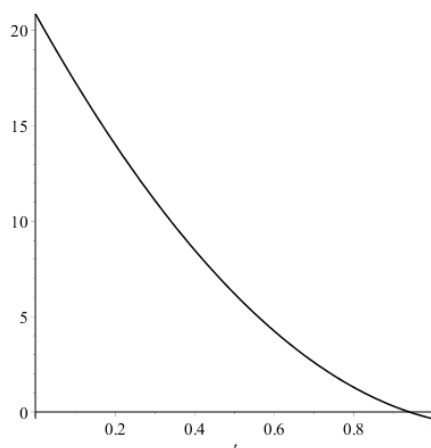


Figure 18. Dendrimer Architecture

#### 4. Conclusion

A topological index is a number associated with a chemical network that links the physio-chemical properties of certain chemical compounds. The connection between the architecture and various bio capabilities, electrochemical stability, and bio activities depends on these graph-matching mathematical values. The summary of the topological index on chemical structure and the associated clinical, chemical, biological, and medicinal properties of drugs may be examined by medical science. In this article, we compute the sixteen irregularity indices  $SHN_t$ . In the last section, we give the graphical representation of  $SHN_t$ .

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