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Data Analysis and Irregularity Measurements in the Identical Structures of Carbon Nanocones CNC_t(m)

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Abstract. Irregularity indices are topological indices by nature. They are highly helpful for determining the quantitative topography of nonregular graphs' molecular structures. Both the quantitative structure-property relationship (QSPR) and the quantitative structure-activity relationship (QSAR) depend heavily on the computation of abnormalities in a graph. It is made up of several chemical and physical characteristics, including resistance, enthalpy, entropy, toxicity, melting and boiling points, and entropy. This paper examines the application of different irregularity indices to identify irregularity measurements (IMs) in the network of carbon nanocone molecules $CNC_t(m)$, for $t = 4, 5$, and t. We have used different irregularity indices such as $\operatorname{Irdif}(\xi_t)$, $\operatorname{Al}(\xi_t)$, $\operatorname{Irl}(\xi_t)$, $\operatorname{Irlu}(\xi_t)$, $\operatorname{Irlf}(\xi_t)$, $\operatorname{Irf}(\xi_t)$, $\operatorname{Irla}(\xi_t)$, $\operatorname{Ird1}(\xi_t)$, $\operatorname{Ira}(\xi_t)$, $\operatorname{Irga}(\xi_t)$, $\operatorname{Irb}(\xi_t)$ & $\operatorname{Irr}_t(\xi_t)$. Comparative graphic measures of irregularity in $CNC_4(m), CNC_5(m)$ and $CNC_t(m)$ have also been examined and presented. We are interested in creating new formulas to gain a better understanding of irregularity measures in carbon nanocones using the indices described above.

2020 Mathematics Subject Classifications: 05C09, 05C10, 05C12, 05C31, 05C07, 05C10, 05C90, 05C92

Key Words and Phrases: Carbon nanocones, graphical measurements, vertex degree, edges, irregularity

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1. Introduction

The most significant and fascinating element in existence is carbon. Without carbon, life on Earth would not be conceivable. It makes up the majority of the body's fats, proteins, carbohydrates, muscular tissue, and DNA. It is a non-metallic molecular component that is produced cosmically when helium burns. Technology based on atoms and molecules is known as nanotechnology. It comprises the design and decision-making involved in creating nanodevices. The use of carbon nanoparticles in nanotechnology [3, 9, 28] is crucial.

Carbon nanocones are structures that are conical in shape. They were invented in 1968 [12, 30]. They are useful for capping thin carbon on ultrafine gold needles that are used in scanning probe microscopy [10, 15, 26]. Carbon nanostructures have various real-life applications, such as biosensors, energy storage, and gas sensors [2, 27]. Carbon nanocones are typically symbolized as $CNC_t(m)$. A topological descriptor (TD) is known as the irregularity index of a graph ξ_t if $(TD(\xi_t) \geq 0$ and $TD(\xi_t) = 0$ iff ξ_t is a regular graph. Many researchers have described that the prediction and discrimination of irregularity indices are low [13, 25, 31]. The main motivation of this study is how irregularity indices give accurate results that are used in many fields like enthalpy and entropy. The irregularity indices [1, 14, 29, 33] are depicted in Table 1.

Irregularity Indices		
$\mathrm{Irr_s}(\xi_t) = \frac{1}{2}\sum_{\rho\mu\in E(\xi_t)} \lvert d_\rho - d_\mu\rvert$	$\mathrm{Ira}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \left(d_\rho^{-\frac{1}{2}} - d_\mu^{-\frac{1}{2}}\right)^2$	$\mathrm{Irga}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \ln \frac{d_\rho + d_\mu}{2\sqrt{d_\rho \times d_\mu}}$
$\mathrm{Al}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \lvert d_\rho - d_\mu\rvert$	$\mathrm{Irdif}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \left\lvert \frac{d_\rho}{d_\mu} - \frac{d_\mu}{d_\rho}\right\rvert^2$	$\mathrm{Irla}(\xi_t) = 2\sum_{\rho\mu\in E(\xi_t)} \frac{\lvert d_\rho - d_\mu\rvert}{d_\rho + d_\mu}$
$\mathrm{Irf}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} (d_\rho - d_\mu)^2$	$\mathrm{Irlu}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \frac{\lvert d_\rho - d_\mu\rvert}{\min(d_\rho, d_\mu)}$	$\mathrm{Ird1}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \ln\{1 + \lvert d_\rho - d_\mu\rvert\}$
$\mathrm{Irb}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \left(d_\rho^{\frac{1}{2}} - d_\mu^{\frac{1}{2}}\right)^2$	$\mathrm{Irlf}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \frac{\lvert d_\rho - d_\mu\rvert}{\sqrt{d_\rho \times d_\mu}}$	$\mathrm{Irl}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \lvert \ln d_\rho - \ln d_\mu\rvert$

Table 1: Irregularity indices for $\xi_t = CNC_t(m)$, for $t = 4, 5$ and t.

2. Material and Methods

Let ξ_t be an undirected, connected, simple, and finite graph of Carbon nanocones where d_ρ and d_μ are the valencies of the nodes ρ and μ, respectively [18, 23]. It is symbolized as $CNC_t(m)$. We take the molecular structures of Carbon nanocones $CNC_t(m)$, for $t = 4, 5$ and t, and then different irregularity indices such as $\mathrm{Irdif}(\xi_t)$, $\mathrm{Al}(\xi_t)$, $\mathrm{Irl}(\xi_t)$, $\mathrm{Irlu}(\xi_t)$, $\mathrm{Irlf}(\xi_t)$, $\mathrm{Irf}(\xi_t)$, $\mathrm{Irla}\ (\xi_t)$, $\mathrm{Ird1}(\xi_t)$, $\mathrm{Ira}(\xi_t)$, $\mathrm{Irga}(\xi_t)$, $\mathrm{Irb}(\xi_t)$ and $\mathrm{Irr}_s(\xi_t)$ are computed. We have used the comparative study method of testing by choosing the different molecular structures of Carbon nanocones. We have applied twelve irregularity indices to four different Carbon nanocones that are $CNC_t(m)$, for $t = 4, 5$ and t. [4, 20].

3. Applications

The above-calculated irregularity descriptors for the chemical compound Carbon nanocones network symbolically represented by $\xi_t = CNC_t(m)$, for $t = 4, 5$ and t, can be used to examine many physiochemical topographies [17, 19, 22]. Some of these topographies are given below:

(i) Standard enthalpy of vaporization (DH_{VAP})

(ii) Boiling point (B_P)

(iii) Density

(iv) Solubility.

(v) Partition Coefficient.

(vi) Ionization.

(vii) Hydrogen Bonding.

(viii) Chelation.

(ix) Isosterism.

(x) Entropy

(xi) Surface activity.

(xii) Enthalpy of vaporization (H_{VAP})

(xiii) Melting point

(xiv) Ionization energy.

Irregularity descriptors describe specific consequences about the above-mentioned chemical features [11, 16, 24]. Irregularity descriptors may support to explore also the chemical, biological, and nano properties that are extensively familiarized in developing parts of any country. Therefore, we calculate irregularity measurements for generalized version of $CNC_t(m), t = 4, 5, \ldots n$ & $m = 1, 2, 3, \ldots n$.

4. Main Results and Discussion

We consider the molecular structures of Carbon nanocones $CNC_t(m)$, for $t = 4, 5$ and t shown in Figures 1-3. Let us choose $CNC_t(m)$ for $t = 4$ i.e., $CNC_4(m)$. We construct its molecular structure and apply different irregularity indices on it to get irregularity measurements. [6, 7, 21].

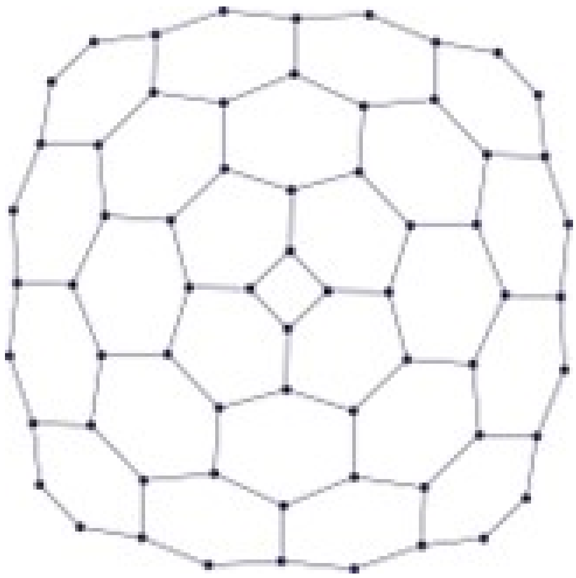


Figure 1: Graphical representation of $\mathrm{CNC}_4(m)$

d_μ	$\lvert V(d_\mu)\rvert$	(d_ρ, d_μ)	$\lvert V(d_\rho, d_\mu)\rvert$
2	$4(m+1)$	$(2,2)$	4
3	$4m^2+4m$	$(2,3)$	$8m$
-	-	$(3,3)$	$2\left(3m^2+m\right)$

Table 2: Depiction of the partition of edges of $\mathrm{CNC}_4(m)$.

With the help of Table 1 and Table 2, we have the following theorems:

Theorem 1 Let ξ_t be the molecular graph of Carbon nanocones $\mathrm{CNC_t(m)}$ with $t=4$, then the irregularity indices are given by:

$$\begin{aligned}
\operatorname{Irdif}(\xi_{t=4}) &= 50/9m \\
\operatorname{Al}(\xi_{t=4}) &= 8m \\
\operatorname{Irl}(\xi_{t=4}) &= 3.2437m \\
\operatorname{Irlu}(\xi_{t=4}) &= 4m \\
\operatorname{Irlf}(\xi_{t=4}) &= 3.2659m \\
\operatorname{Irf}(\xi_{t=4}) &= 8m \\
\operatorname{Irla}(\xi_{t=4}) &= 3.2m \\
\operatorname{Ird}1(\xi_{t=4}) &= 5.5451m \\
\operatorname{Ira}(\xi_{t=4}) &= 0.1346m \\
\operatorname{Irga}(\xi_{t=4}) &= 0.1632m \\
\operatorname{Irb}(\xi_{t=4}) &= 0.8081m \\
\operatorname{Ir} r_s(\xi_{t=4}) &= 4m
\end{aligned}$$

Proof. The cardinality of $\xi_{t=4}$ with respect to the vertices is $|V(\xi_{t=4})| = 4(m+1)^2$ and the cardinality of $\xi_{t=4}$ with respect to the edges is $|E(\xi_{t=4})| = 2\left(3m^2+5m+2\right)$. For this graph we identify $(2,2),(2,3)$ and $(3,3)$ types of edges.

$$\operatorname{Irdif}(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_{t=4})} \left|\frac{d_\rho}{d_\mu} - \frac{d_\mu}{d_\rho}\right| = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)\left|\frac{d_\rho}{d_\mu} - \frac{d_\mu}{d_\rho}\right| = 6.67m.$$

$$Al(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_{t=4})} |d_\rho - d_\mu| = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)|d_\rho - d_\mu| = 8m.$$

$$\operatorname{Irl}(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_t)} |\ln d_\rho - \ln d_\mu| = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)|\ln d_\rho - \ln d_\mu| = 3.243m.$$

$$\operatorname{Irlu}(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_t)} \frac{|d_\rho - d_\mu|}{\min(d_\rho, d_\mu)} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \ddots; \frac{|d_\rho - d_\mu|}{\min(d_\rho, d_\mu)} = 4 \text{ m}.$$

$$\operatorname{Irlf}(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_t)} \frac{|d_\rho - d_\mu|}{\sqrt{d_\rho \times d_\mu}} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)\frac{|d_\rho - d_\mu|}{\sqrt{d_\rho \times d_\mu}} = 3.2659 \text{ m}.$$

$$\operatorname{Irf}(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_t)} (d_\rho - d_\mu)^2 = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)(d_\rho - d_\mu)^2 = 8m.$$

$$\operatorname{Irla}(\xi_{t=4}) = 2\sum_{\rho\mu\in E(\xi_t)} \frac{|d_\rho - d_\mu|}{d_\rho + d_\mu} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)\frac{|d_\rho - d_\mu|}{d_\rho + d_\mu} = 3.2m.$$

$$\operatorname{Ird1}(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_t)} \ln\{1 + |d_\rho - d_\mu|\} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)\ln\{1 + |d_\rho - d_\mu|\} = 5.5451 \text{ m}.$$

$$\operatorname{Ira}(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_t)} \left(d_\rho^{-\frac{1}{2}} - d_\mu^{-\frac{1}{2}}\right)^2 = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)\left(d_\rho^{-\frac{1}{2}} - d_\mu^{-\frac{1}{2}}\right)^2 = 0.1346m.$$

$$\operatorname{Irga}(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_t)} \ln\frac{d_\rho + d_\mu}{2\sqrt{d_\rho \times d_\mu}} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)\ln\frac{d_\rho + d_\mu}{2\sqrt{d_\rho \times d_\mu}} = 0.1632 \text{ m}.$$

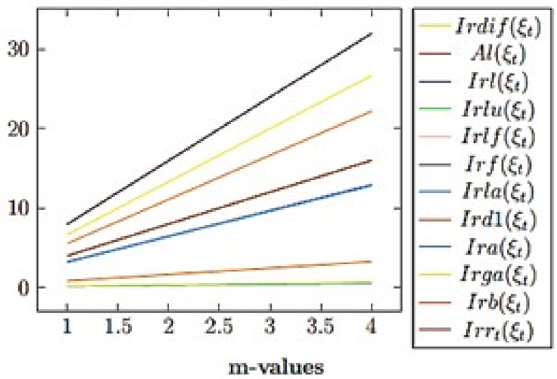
$$\operatorname{Irb}(\xi_{t=4}) = \sum_{\rho\mu\in E(\xi_t)} \left(d_\rho^{\frac{1}{2}} - d_\mu^{\frac{1}{2}}\right)^2 = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)\left(d_\rho^{\frac{1}{2}} - d_\mu^{\frac{1}{2}}\right)^2 = 0.8081 \text{ m}.$$

$$\operatorname{Irr}_s(\xi_{t=4}) = \frac{1}{2}\sum_{\rho\mu\in E(\xi_t)} |d_\rho - d_\mu| = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})}\right)|d_\rho - d_\mu| = 4m.$$

All irregularity measurements for the Carbon nanocones network $CNC_4(m)$ by using the test values of parameter t, are shown in Table 3.

Irregularity Indices	$m=1$	$m=2$	$m=3$	$m=4$
Irdif (ξ_t)	5.58	11.12	16.68	22.24
Al (ξ_t)	8	16	24	32
Irl (ξ_t)	3.24	6.49	9.73	12.97
Irlu (ξ_t)	4	8	12	16
Irlf (ξ_t)	3.27	6.53	9.80	13.06
Irf (ξ_t)	8	16	24	32
Irla (ξ_t)	3.20	6.40	9.60	12.8
Ird 1 (ξ_t)	5.55	11.10	16.65	22.2
Ira (ξ_t)	0.13	0.27	0.40	0.54
Irga (ξ_t)	0.16	0.33	0.49	0.65
Irb (ξ_t)	0.81	1.62	2.42	3.23
Irr (ξ_t)	4	8	12	16

Table 3: Depiction of irregularity indices with some test values for $\xi_4 = \mathrm{CNC}_4(\mathrm{~m})$.



Graph I: Graphical Measurements of irregularity in $\mathrm{CNC}_4(\mathrm{m})$.

Now, let us choose $CNC_t(m)$ for $t=5$ i.e., $CNC_5(m)$. We construct its molecular structure and apply different irregularity indices to obtain irregularity measurements.

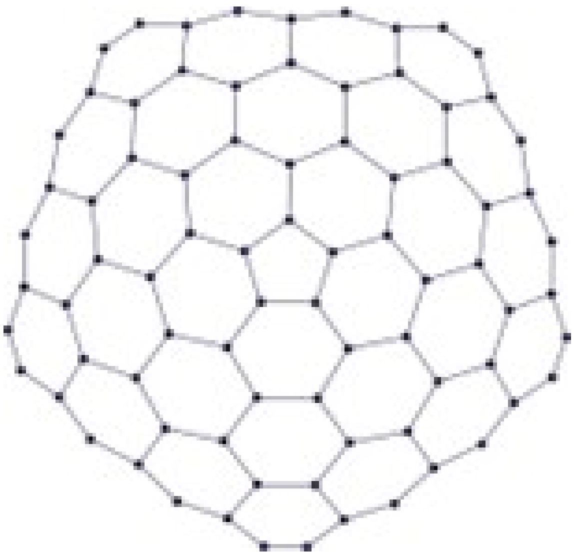


Figure 2: Molecular depiction of $CNC_5(\text{ m})$

d_μ	$\|V(d_\mu)\|$	(d_ρ, d_μ)	$\|V(d_\rho, d_\mu)\|$
2	$5(m+1)$	$(2,2)$	5
3	$5m^2+5m$	$(2,3)$	$10m$
-	-	$(3,3)$	$2.5\left(3m^2+m\right)$

Table 4: Depiction of the partition of edges of $\mathrm{CNC}_5(\text{ m})$.

With the help of Table 1 and Table 4, we have the following theorems.

Theorem 2. Let ξ_t be the molecular graph of Carbon nanocones $\mathrm{CNC_t(m)}$ with $t=5$, then the irregularity indices are given by:

$$\begin{aligned}
\operatorname{Irdif}(\xi_{t=5}) &= 6.94 \text{ m}\\
\operatorname{Al}(\xi_{t=5}) &= 10 \text{ m}\\
\operatorname{Irl}(\xi_{t=5}) &= 4.0546 \text{ m}\\
\operatorname{Irlu}(\xi_{t=5}) &= 5 \text{ m}\\
\operatorname{Irlf}(\xi_{t=5}) &= 4.0824 \text{ m}\\
\operatorname{Irf}(\xi_{t=5}) &= 10 \text{ m}\\
\operatorname{Irla}(\xi_{t=5}) &= 4 \text{ m}\\
\operatorname{Ird1}(\xi_{t=5}) &= 6.9314 \text{ m}\\
\operatorname{Ira}(\xi_{t=5}) &= 0.1683 \text{ m}\\
\operatorname{Irga}(\xi_{t=5}) &= 0.2041 \text{ m}\\
\operatorname{Irb}(\xi_{t=5}) &= 1.0102 \text{ m}\\
\operatorname{Ir}_s(\xi_{t=5}) &= 5 \text{ m}.
\end{aligned}$$

Proof. The cardinality of $\xi_{t=5}$ with respect to the vertices is $|V(\xi_{t=5})| = 5(m+1)^2$ and the cardinality of $\xi_{t=5}$ with respect to the edges is $|E(\xi_{t=5})| = \frac{5}{2}\left(3m^2+5m+2\right)$. We have found $(2,2)$, $(2,3)$ and $(3,3)$ types of edges.

$$\operatorname{Irdif}(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_{t=4})} \left| \frac{d_\rho}{d_\mu} - \frac{d_\mu}{d_\rho} \right| = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} \vdots; \right) \left| \frac{d_\rho}{d_\mu} - \frac{d_\mu}{d_\rho} \right| = 8.33 \text{ m.}$$

$$Al(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_{t=4})} |d_\rho - d_\mu| = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} \right) |d_\rho - d_\mu| = 10 \text{ m.}$$

$$\operatorname{Irl}(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_t)} |\ln d_\rho - \ln d_\mu| = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} \bar{i} \right) |\ln d_\rho - \ln d_\mu| = 4.0546m.$$

$$\operatorname{Irlu}(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_t)} \frac{|d_\rho - d_\mu|}{\min(d_\rho, d_\mu)} = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} \right) \frac{|d_\rho - d_\mu|}{\min(d_\rho, d_\mu)} = 5 \text{ m.}$$

$$\operatorname{Irlf}(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_t)} \frac{|d_\rho - d_\mu|}{\sqrt{d_\rho \times d_\mu}} = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} \right) \frac{|d_\rho - d_\mu|}{\sqrt{d_\rho \times d_\mu}} = 4.0824 \text{ m.}$$

$$\operatorname{Irf}(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_t)} (d_\rho - d_\mu)^2 = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} \right) (d_\rho - d_\mu)^2 = 10 \text{ m.}$$

$$\operatorname{Irla}(\xi_{t=5}) = 2 \sum_{\rho\mu \in E(\xi_t)} \frac{|d_\rho - d_\mu|}{d_\rho + d_\mu} = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} ; \frac{|d_\rho - d_\mu|}{d_\rho + d_\mu} = 4m. \right.$$

$$\operatorname{Ird1}(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_t)} \ln\{1 + |d_\rho - d_\mu|\} = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} ; \ln\{1 + |d_\rho - d_\mu|\} \right.$$
$$= 6.9314 \text{ m.}$$

$$\operatorname{Ira}(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_t)} \left(d_\rho^{-\frac{1}{2}} - d_\mu^{-\frac{1}{2}} \right)^2 = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} \right) \left(d_\rho^{-\frac{1}{2}} - d_\mu^{-\frac{1}{2}} \right)^2 = 0.1683m.$$

$$\operatorname{Irga}(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_t)} \ln \frac{d_\rho + d_\mu}{2\sqrt{d_\rho \times d_\mu}} = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} \vdots \ln \frac{d_\rho + d_\mu}{2\sqrt{d_\rho \times d_\mu}} = 0.2041 \text{ m.} \right.$$

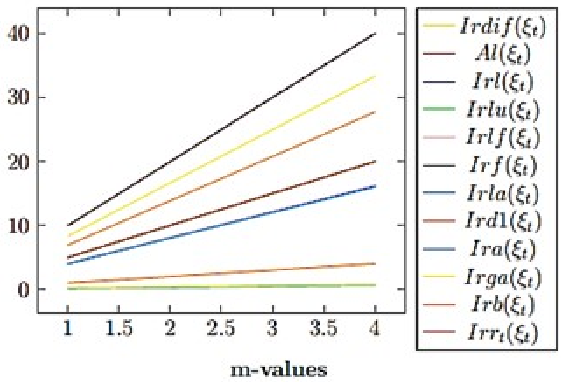
$$\operatorname{Irb}(\xi_{t=5}) = \sum_{\rho\mu \in E(\xi_t)} \left(d_\rho^{\frac{1}{2}} - d_\mu^{\frac{1}{2}} \right)^2 = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} \right) \left(d_\rho^{\frac{1}{2}} - d_\mu^{\frac{1}{2}} \right)^2 = 1.0102m.$$

$$\operatorname{Irr}_s(\xi_{t=5}) = \frac{1}{2} \sum_{\rho\mu \in E(\xi_t)} |d_\rho - d_\mu| = \left(\sum_{\rho\mu \in E^{22}(\xi_{t=4})} + \sum_{\rho\mu \in E^{23}(\xi_{t=4})} + \sum_{\rho\mu \in E^{33}(\xi_{t=4})} ; d_\rho - d_\mu \mid = 5m. \right.$$

All irregularity measurements for the Carbon nanocones network CNC_5(m) by using test values of parameter t, are shown in Table 5.

Irregularity Indices	$m=1$	$m=2$	$m=3$	$m=4$
Irdif (ξ_t)	6.94	13.88	20.80	27.76
Al (ξ_t)	10	20	30	40
Irl (ξ_t)	4.05	8.10	12.15	16.2
Irlu (ξ_t)	5	10	15	20
Irlf (ξ_t)	4.08	8.16	12.24	16.32
Irf (ξ_t)	10	20	30	40
Irla (ξ_t)	4	8	12	16
Ird1 (ξ_t)	6.93	13.86	20.79	27.72
Ira (ξ_t)	0.17	0.34	0.51	0.68
Irga (ξ_t)	0.20	0.40	0.60	0.80
Irb (ξ_t)	1.01	2.02	3.03	4.04
Irr r_t (ξ_t)	5	10	15	20

Table 5: Depiction of irregularity indices with some test values for $\xi_5 = CNC_5($ m$)$.



Graph2: Graphical Measurements of irregularity in $CNC_5($ m$)$.

Now, let us choose $CNC_t(m)$ for $t = t$ i.e., $CNC_t(m)$. We construct its molecular structure and apply different irregularity indices to obtain irregularity measurements.

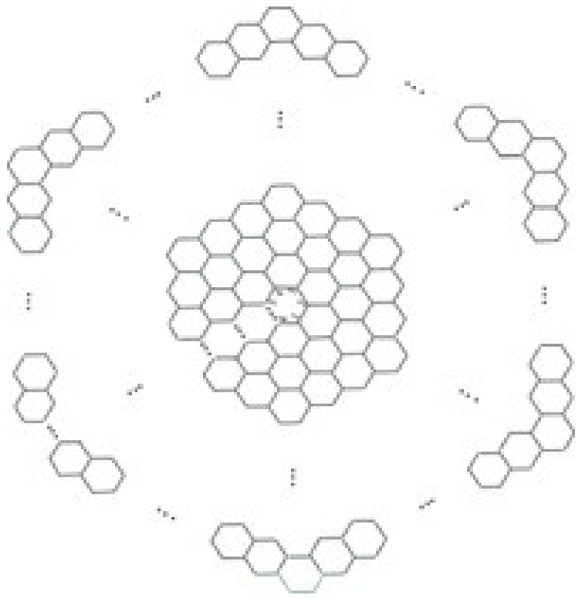


Figure 3: Graphical formation display of generalized form of $\mathrm{CNC}_t($ m)

d_μ	$\|V(d_\mu)\|$	(d_ρ, d_μ)	$\|V(d_\rho, d_\mu)\|$
2	$t(m+1)$	$(2,2)$	t
3	$t\left(m^2+m\right)$	$(2,3)$	$2tm$
-	-	$(3,3)$	$0.5t\left(3m^2+m\right)$

Table 6: Depiction of the partition of edges of $CNC_t(m)$.

With the help of Table 1 and Table 6, we have the following theorems.

Theorem 3. Let ξ_{t} be the molecular graph of Carbon nanocones $\mathrm{CNC_t(m)}$ with $t=t$, then the irregularity indices are given by:

$$\begin{gathered}
\operatorname{Irdif}\left(\xi_t\right)=1.3888 \mathrm{tm} \\
\operatorname{Al}\left(\xi_t\right)=2 \mathrm{tm} \\
\operatorname{Irl}\left(\xi_t\right)=0.8109 \mathrm{tm} \\
\operatorname{Irlu}\left(\xi_t\right)=\mathrm{tm} \\
\operatorname{Irlf}\left(\xi_t\right)=0.8164 \mathrm{tm} \\
\operatorname{Irf}\left(\xi_t\right)=2 \mathrm{tm} \\
\operatorname{Irla}\left(\xi_t\right)=0.4 \mathrm{tm} \\
\operatorname{Ird} 1\left(\xi_t\right)=1.3862 \mathrm{tm} \\
\operatorname{Ira}\left(\xi_t\right)=0.0336 \mathrm{tm} \\
\operatorname{Irga}\left(\xi_t\right)=0.0408 \mathrm{tm} \\
\operatorname{Irb}\left(\xi_t\right)=0.2020 \mathrm{tm} \\
\operatorname{Irr}\left(\xi_t\right)=\mathrm{tm}
\end{gathered}$$

Proof. The cardinality of ξ_t with respect to the vertices is $\left|V\left(\xi_t\right)\right| = t(m+1)^2$ and the cardinality of ξ_t with respect to the edges is $\left|E\left(\xi_t\right)\right| = \frac{t}{2}\left(3m^2+5m+2\right)$. We have found $(2,2),(2,3)$ and $(3,3)$ types of edges.

$$\operatorname{Irdif}(\xi_t) = \sum_{\rho\mu\in E(\xi_{t=4})} \left|\frac{d_\rho}{d_\mu} - \frac{d_\mu}{d_\rho}\right| = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \vdots \right) \left|\frac{d_\rho}{d_\mu} - \frac{d_\mu}{d_\rho}\right| = 1.6666\text{tm}.$$

$$Al(\xi_t) = \sum_{\rho\mu\in E(\xi_{t=4})} |d_\rho - d_\mu| = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \right) |d_\rho - d_\mu| = 2\text{tm}.$$

$$\operatorname{Irl}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} |\ln d_\rho - \ln d_\mu| = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \vdots \right) |\ln d_\rho - \ln d_\mu| = 0.8109\text{tm}.$$

$$\operatorname{Irlu}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \frac{|d_\rho - d_\mu|}{\min(d_\rho, d_\mu)} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} ; \right) \frac{|d_\rho - d_\mu|}{\min(d_\rho, d_\mu)} = tm.$$

$$\operatorname{Irlf}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \frac{|d_\rho - d_\mu|}{\sqrt{d_\rho \times d_\mu}} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \right) \frac{|d_\rho - d_\mu|}{\sqrt{d_\rho \times d_\mu}} = 0.8164\text{tm}.$$

$$\operatorname{Irf}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} (d_\rho - d_\mu)^2 = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \right) (d_\rho - d_\mu)^2 = 2\text{tm}.$$

$$\operatorname{Irla}(\xi_t) = 2\sum_{\rho\mu\in E(\xi_t)} \frac{|d_\rho - d_\mu|}{d_\rho + d_\mu} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \right) \frac{|d_\rho - d_\mu|}{d_\rho + d_\mu} = 0.8\text{tm}.$$

$$\operatorname{Ird1}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \ln\{1 + |d_\rho - d_\mu|\} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} ; \ln\{1 + |d_\rho - d_\mu|\} = 1.3862\text{tm}.\right.$$

$$\operatorname{Ira}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \left(d_\rho^{-\frac{1}{2}} - d_\mu^{-\frac{1}{2}}\right)^2 = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \right) \left(d_\rho^{-\frac{1}{2}} - d_\mu^{-\frac{1}{2}}\right)^2 = 0.0336\text{tm}.$$

$$\operatorname{Irga}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \ln\frac{d_\rho + d_\mu}{2\sqrt{d_\rho \times d_\mu}} = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \right) \ln\frac{d_\rho + d_\mu}{2\sqrt{d_\rho \times d_\mu}} = 0.0408\text{tm}.$$

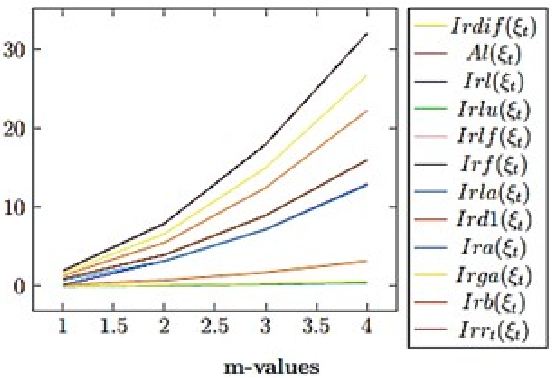
$$\operatorname{Irb}(\xi_t) = \sum_{\rho\mu\in E(\xi_t)} \left(d_\rho^{\frac{1}{2}} - d_\mu^{\frac{1}{2}}\right)^2 = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} \right) \left(d_\rho^{\frac{1}{2}} - d_\mu^{\frac{1}{2}}\right)^2 = 0.2020tm.$$

$$\operatorname{Irr}_s(\xi_t) = \frac{1}{2}\sum_{\rho\mu\in E(\xi_t)} |d_\rho - d_\mu| = \left(\sum_{\rho\mu\in E^{22}(\xi_{t=4})} + \sum_{\rho\mu\in E^{23}(\xi_{t=4})} + \sum_{\rho\mu\in E^{33}(\xi_{t=4})} |d_\rho - d_\mu| = tm\right.$$

All irregularity measurements for the Carbon nanocones network $CNC_t(m)$ by using test values of parameter m, are shown in Table 7 with their graphical representation in graph 3 .

Irregularity Indices	$m=1$	$m=2$	$m=3$	$m=4$
Irdif (ξ_t)	1.39 t	2.78 t	5.01 t	5.56 t
Al (ξ_t)	2 t	4 t	6 t	8 t
Irl (ξ_t)	0.81 t	1.62 t	2.43 t	3.24 t
Irlu (ξ_t)	t	2 t	3 t	4 t
Irlf (ξ_t)	0.82 t	1.64 t	2.46 t	3.28 t
Irf (ξ_t)	2 t	4 t	6 t	8 t
Irla (ξ_t)	0.4 t	0.8 t	1.2 t	1.6 t
Ird1 (ξ_t)	1.39 t	2.78 t	4.17 t	5.56 t
Ira (ξ_t)	0.03 t	0.06 t	0.09 t	0.12 t
Irga (ξ_t)	0.04 t	0.08 t	0.12 t	0.16 t
Irb (ξ_t)	0.20 t	0.40 t	0.60 t	0.80 t
Irr t (ξ_t)	t	2 t	3 t	4 t

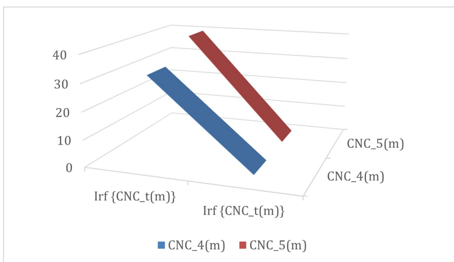
Table 7: Depiction of irregularity indices with some test values for $\xi_t = CNC_t(m)$.



Graph 3: Graphical Measurements of irregularity in $CNC_{t=1}(m)$.

	Irf (ξ_t)	Ira (ξ_t)
$CNC_4($ m$)$	32	0.54
$CNC_5($ m$)$	40	0.68

Table 8: Shows the irregularity indices Irf (ξ_t) and Ira (ξ_t) for $\xi_t = CNC_{t=4,5}($ m$)$.



Graph4: Graphical Analysis of irregularity in $CNC_{t=4,5}($ m$)$.

IMs	$CNC_t(m), t = 4, 5, \ldots n\&m = 1, 2, 3, \ldots n$
Irdif (ξ_t)	1.39 tm
Al (ξ_t)	2 tm
Irl (ξ_t)	0.81 tm
Irlu (ξ_t)	tm
Irlf (ξ_t)	0.82 tm
Irf (ξ_t)	2 tm
Irla (ξ_t)	$0.40tm$
Ird 1 (ξ_t)	1.39 tm
Ira (ξ_t)	0.03 tm
Irga (ξ_t)	$0.04t$tm
Irb (ξ_t)	0.20 tm
Irr $r_s)$	tm

Table 9: Shows the irregularity measurements with generalized form of Carbon nancones.

5. Conclusion

We analyse the theoretical and graphical data we acquired for the Carbon Nanocones network $CNC_t(m)$, for $t = 4, 5$ and t using the twelve irregularity indices described above. Based on these results, we determine which molecular network is more irregular than the others according to a certain irregularity index. It has been noted that, for $CNC_t(m)$, for $t = 4, 5$ and t, all of the generated graphs have a straight-line form, and all formulas derived from irregularity indices are linear in m and $CNC_t($ m) are dependent on a parameter m . It has shown that increasing the parameter value causes the irregularity indices' value to grow as well. Graphs 1-2 show the graphic behaviour of IM for $CNC_t(m)$, for $t = 4, 5$.
The calculated and shown irregularity indices for for $\xi_t = CNC_{t=4,5,}($ m) are presented in Table 8. The irregularity measurements for the generalized version of of $CNC_t(m), t = 4, 5, \ldots n\&$ $m = 1, 2, 3, \ldots n$, are displayed in Table 9. The graphical behaviour of $CNC_4(m)$, $CNC_5(m)$ for the irregularity index Ir f (ξ_t) is shown by the black line.On the other hand, graph 4 shows the graphical behavior of $CNC_4($ m$), CNC_5($ m) for the irregularity index Ira (ξ_t), as represented by the pink line.
Moreover, a variety of physiochemical parameters, including those listed in Section 5 above, can be found and compared using irregularity indices [5, 8, 32]. Using irregularity indices, correlation, and the regression model $P = a + bX$, where X can be any topological index - we determine the experimental values of the fourteen physiochemical parameters listed above and then compare them to our estimated values. Additionally, we can contrast their major and non-significant errors. If we compute the fourteen physiochemical parameters listed above more accurately and numerically using irregularity indices, we do not require the experimental results.

It has also been observed that the difference of irregularity measurements for Irf (ξ_t)

among $CNC_4(\text{ m})$ and $CNC_5(\text{ m})$ are unified. Similarly, the difference of irregularity measurements for Ira (ξ_t) among $CNC_4(\text{ m})$ and $CNC_5(\text{ m})$ are same.

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Data Availability: All data used are included inside the manuscript.

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