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Entropy Measures of $g - C_3N_5$ using Topological Indices

E. Lavanya, M. A. Sriraj and P. Siva Kota Reddy

ABSTRACT: Topological descriptors are non-empirical numerical quantities that characterise molecular structures. These descriptors are essential to the QSAR/QSPR approaches, as they provide theoretical chemists with a basis for investigating and synthesising chemical structures. Entropic measures are a type of topological descriptors that have many applications, ranging from the quantitative description of a chemical structure to the investigation of specific chemical properties of molecular graphs. Shannon's entropy metrics characterise graphs and networks by analysing their structural information. This study is mainly concerned with the computation of analytical expressions for degree-based entropy metrics for the chemical graph of $g - C_3N_5$. In addition to shedding light on the relationship between entropy measures and molecular structure, the numerical results of the entropy measures derived in this paper cast light on the relationship between entropy measures and molecular structure.

Key Words: Topological indices, Degree-based entropy, $g - C_3N_5$.

Contents

1. Introduction

In modelling chemical graphs, graph theory plays an important role. Various characteristics, including physical, chemical and biological activities are analysed through the use of graph theory applications. These properties are evaluated using topological indices, which are numerical invariants. The topological index defines the physicochemical and biological properties of a graph. QSAR and QSPR use structural, exploratory, factors to simulate a particular characteristic, typically through a weighted combination of these parameters. Considering the connection between atoms in structure, geometry, and molecular framework as the ultimate origin of any property, if the number of molecules in the subject's study set is sufficient and the structural characteristics are precise enough then any desired characteristic can be predicted using only the study set's structural parameters.

Entropy-based methods are potent tools for studying a variety of problems in fields such as mathematical pattern recognition, robotics, mathematical physics and chemistry. In chemical graph theory for instance, there are numerous methods for characterizing the structures based on well known topological indices that can be seen in [1]. Determining the structural information content of a graph is another typical problem in the aforementioned fields. Finding a particular division of the vertex set in order to obtain a probability distribution is the mainstay of classical approaches for computing the structural information regard to a graph. The idea of graph entropy, which was proposed by Rashevsky and Trucco, is utilised to measure the structure's structural complexity, of graphs [3]. Mowshowitz [10] first explained the entropy of a graph as an information-theoretic quantity. Here, the complexity of a graph

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is determined by the well-known Shannon entropy. Entropic network measures are used to quantify a molecular structure and examine its chemical characteristics. We recommend that the reader read the works [8,9,11-15,18-21,23,25] for new topological indices.

In recent years, chemists and physicists have studied numerous graphitic carbon nitrides (g-CNs) primarily to reduce the band gap and reach improved chemical and physical properties. The $g-C_3N_5$ class of molecules which has a larger nitrogen content than $g-C_3N_4$, possesses superior electronic features including a reduced band gap and catalytic capabilities among others. In this study the computaion of entropy measures for $g-C_3N_5$ using the topological indices 1^{st} Zagreb, 2^{nd} Zagreb, 3^{rd} Zagreb, Atom bond connectivity, Geometric-arithmetic, Arithmetic-geometric, Forgotten, Harmonic and Randić indices.

2. Degree Based Indices of Graphs

Examining the structural-dependence of total-electron energy, a formula in terms of Zagreb indices $M_1(G)$ and $M_2(G)$ [7] occured

$$M_1(G) = \sum_{pq \in E(G)} (d_p + d_q)$$

and

$$M_2(G) = \sum_{pq \in E(G)} (d_p \times d_q).$$

Fath-Tabar found the Third Zagreb index of a graph G in [6] as

$$ZG_3(G) = \sum_{pq \in E(G)} |d_p - d_q|.$$

The Atom-bond Connectivity index is contributed by Estrada et al. in [4] as

$$ABC(G) = \sum_{pq \in E(G)} \sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}}.$$

ABC-index has a strong correlation with the thermodynamic features of alkanes, particularly their temperatures of formation.

The Geometric-arithmetic index of a graph is established by Vukicevic et al. in [27] as

$$GA(G) = \sum_{pq \in E(G)} \frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q}.$$

Besides mathematical studies of the GA index, chemists are interested in its applicability to acyclic, unicyclic, and bicyclic molecular graphs, benzenoid hydrocarbons, and phenylenes.

The inverse invariant of Geometric-arithmetic index is introduced in [26], as

$$AG(G) = \sum_{pq \in E(G)} \frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}}.$$

Furtula and Gutman [5] contributed the Forgotten index as

$$F(G) = \sum_{pq \in E(G)} ({d_p}^2 + {d_q}^2).$$

Gao and Wang presented the general Harmonic index in [28] as

$$H_k(G) = \sum_{pq \in E(G)} \left(\frac{2}{d_p + d_q} \right)^k .$$

Further by taking $k = 1$ in general Harmonic index, we get the normal harmonic index is given as

$$H(G) = \sum_{pq \in E(G)} \frac{2}{(d_p + d_q)}.$$

The Randić index proved instantly suitable for drug design and was utilised several times. Ballobas and Erdos introduced the general Randić index in [22] as

$$R_\alpha(G) = \sum_{pq \in E(G)} (d_p \cdot d_q)^\alpha.$$

3. Edge Weight and Degree Based Entropy of Topological Indices

Let $G = (V(G), E(G), \psi(G))$ be an edge weighted graph, where $V(G)$ is vertex set, $E(G)$ be the edge set, $\psi(G)$ denote the edge weight of edge (pq) respectively. Then the Shannon entropy of edge weighted graph in [24] is represented in below equation:

$$ENT_\psi(G) = - \sum_{p'q' \in E(G)} \frac{\psi(p'q')}{\sum_{pq \in E(G)} \psi(pq)} \log \left[\frac{\psi(p'q')}{\sum_{pq \in E(G)} \psi(pq)} \right].$$

- **The First Zagreb Entropy**
  If $\psi(pq) = (d_p + d_q)$, then

  $$\sum_{pq \in E(G)} \psi(pq) = \sum_{pq \in E(G)} (d_p + d_q) = M_1(G).$$

  and hence the First Zagreb entropy equation reduces to the following form:

  $$ENT_{M_1}(G) = \log(M_1(G)) - \frac{1}{M_1(G)} \log \left[\prod_{pq \in E(G)} [d_p + d_q]^{[d_p + d_q]} \right].$$

- **The Second Zagreb Entropy**
  If $\psi(pq) = (d_p \times d_q)$, then

  $$\sum_{pq \in E(G)} \psi(pq) = \sum_{pq \in E(G)} (d_p \times d_q) = M_2(G)$$

  and hence the Second Zagreb entropy equation reduces to the following form:

  $$ENT_{M_2}(G) = \log(M_2(G)) - \frac{1}{M_2(G)} \log \left[\prod_{pq \in E(G)} [d_p \times d_q]^{[d_p \times d_q]} \right].$$

- **The Third Zagreb Entropy**
  If $\psi(pq) = |d_p - d_q|$, then

  $$\sum_{pq \in E(G)} \psi(pq) = \sum_{pq \in E(G)} |d_p - d_q| = ZG_3(G)$$

  and hence the Third Zagreb entropy equation reduces to the following form:

  $$ENT_{ZG_3}(G) = \log(ZG_3(G)) - \frac{1}{ZG_3(G)} \log \left[\prod_{pq \in E(G)} |d_p - d_q|^{|d_p - d_q|} \right].$$

- **The Atom-Bond Connectivity Entropy**
  If $\psi(pq) = \sqrt{\frac{d_p+d_q-2}{d_p \cdot d_q}}$, then

$$\sum_{pq\in E(G)} \psi(pq) = \sum_{pq\in E(G)} \sqrt{\frac{d_p+d_q-2}{d_p \cdot d_q}} = ABC(G)$$

and hence the Atom-bond connectivity entropy equation reduces to the following form:

$$ENT_{ABC}(G) = \log(ABC(G)) - \frac{1}{ABC(G)} \log\left[\prod_{pq\in E(G)} \left[\sqrt{\frac{d_p+d_q-2}{d_p \cdot d_q}}\right]^{\left[\sqrt{\frac{d_p+d_q-2}{d_p \cdot d_q}}\right]}\right].$$

- **The Geometric-Arithmetic Entropy**
  If $\psi(pq) = \frac{2\sqrt{d_p \cdot d_q}}{d_p+d_q}$, then

$$\sum_{pq\in E(G)} \psi(pq) = \sum_{pq\in E(G)} \frac{2\sqrt{d_p \cdot d_q}}{d_p+d_q} = GA(G)$$

and hence the Geometric-arithmetic entropy equation reduces to the following form:

$$ENT_{GA}(G) = \log(GA(G)) - \frac{1}{GA(G)} \log\left[\prod_{pq\in E(G)} \left[\frac{2\sqrt{d_p \cdot d_q}}{d_p+d_q}\right]^{\left[\frac{2\sqrt{d_p \cdot d_q}}{d_p+d_q}\right]}\right].$$

- **The Arithemetic-Geometric Entropy**
  If $\psi(pq) = \frac{d_p+d_q}{2\sqrt{d_p \cdot d_q}}$, then

$$\sum_{pq\in E(G)} \psi(pq) = \sum_{pq\in E(G)} \frac{d_p+d_q}{2\sqrt{d_p \cdot d_q}} = AG(G)$$

and hence the Arithmetic-geometric entropy equation reduces to the following form:

$$ENT_{AG}(G) = \log(AG(G)) - \frac{1}{AG(G)} \log\left[\prod_{pq\in E(G)} \left[\frac{d_p+d_q}{2\sqrt{d_p \cdot d_q}}\right]^{\left[\frac{d_p+d_q}{2\sqrt{d_p \cdot d_q}}\right]}\right].$$

- **The Forgotten Entropy**
  If $\psi(pq) = [{d_p}^2 + {d_q}^2]$, then

$$\sum_{pq\in E(G)} \psi(pq) = \sum_{pq\in E(G)} [{d_p}^2 + {d_q}^2] = F(G)$$

and hence the Forgotten entropy equation reduces to the following form:

$$ENT_F(G) = \log(F(G)) - \frac{1}{F(G)} \log\left[\prod_{pq\in E(G)} [{d_p}^2 + {d_q}^2]^{[{d_p}^2 + {d_q}^2]}\right].$$

- **The Harmonic Entropy**
  If $\psi(pq) = \frac{2}{(d_p+d_q)}$, then

$$\sum_{pq\in E(G)} \psi(pq) = \sum_{pq\in E(G)} \frac{2}{(d_p+d_q)} = H(G)$$

and hence the Harmonic entropy equation reduces to the following form:

$$ENT_H(G) = \log(H(G)) - \frac{1}{H(G)} \log\left[\prod_{pq\in E(G)} \left[\frac{2}{(d_p+d_q)}\right]^{\left[\frac{2}{(d_p+d_q)}\right]}\right].$$

- **The Randić Entropy**
  If $\psi(pq) = (d_p \cdot d_q)^\alpha$, then

$$\sum_{pq\in E(G)} \psi(pq) = \sum_{pq\in E(G)} (d_p \cdot d_q)^\alpha = R_\alpha(G)$$

and hence the Randić entropy equation reduces to the following form:

$$ENT_{R_\alpha}(G) = \log(R_\alpha(G)) - \frac{1}{R_\alpha(G)} \log\left[\prod_{pq\in E(G)} [(d_p \cdot d_q)^\alpha]^{[(d_p\cdot d_q)^\alpha]}\right].$$

4. Results for the Structure of $g - C_3N_5$

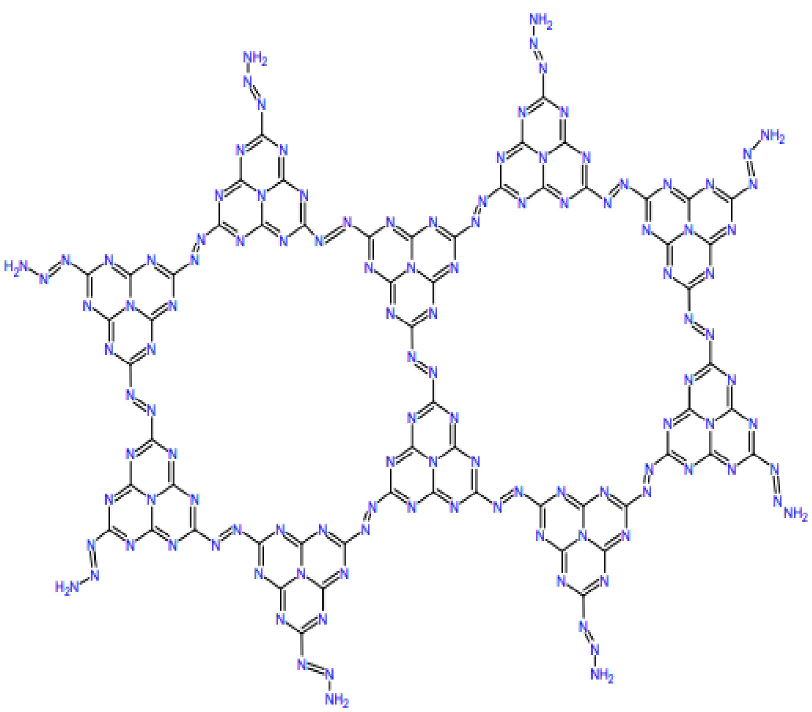

Figure 1: structure of $g - C_3N_5$

From the structure of Graphite Carbon Nitride $g - C_3N_5$, there are $32mn + 2m + 2n$ vertices. In which $2(m+n)$ vertices are of degree 1, $18mn$ vertices are of degree 2 and $14mn$ vertices of degree 3. Here,

m and n represents the total number of Polyaromatic hexagons ($m = n$) in every linear chain joined together by a $N = N$ atoms. Total number of edges are $39mn + m + n$, the edge partition of $g - C_3N_5$ based on degree end vertices are as follows:

Table 1: Edge partition

(d_p, d_q)	number of edges
$(1,2)$	$2(m+n)$
$(2,2)$	$3mn - m - n$
$(2,3)$	$30mn$
$(3,3)$	$6mn$

This section contains the computations of entropies of $g - C_3N_5$.

- **The First Zagreb Entropy of** $g - C_3N_5$
  From the definition of First Zagreb index and edge partition, we get $M_1(G) = 198mn + 2m + 2n$. Applying the First Zagreb entropy equation, we get the following result as

$$
\begin{aligned}
ENT_{M_1(G)} &= \log(M_1(G)) - \frac{1}{M_1(G)} \log\Bigg[\prod_{pq\in E_1} (d_p + d_q)^{(d_p+d_q)} \times \prod_{pq\in E_2} (d_p + d_q)^{(d_p+d_q)} \\
&\quad \times \prod_{pq\in E_3} (d_p + d_q)^{(d_p+d_q)} \times \prod_{pq\in E_4} (d_p + d_q)^{(d_p+d_q)}\Bigg] \\
&= \log(M_1(G)) - \frac{1}{M_1(G)} \log\Bigg[\Big(2(m+n)(3)^{(3)}\Big) \times \Big((3mn - m - n)(4)^{(4)}\Big) \times \\
&\quad \Big((30mn)(5)^{(5)}\Big) \times \Big((6mn)(6)^{(6)}\Big)\Bigg] \\
&= \log(198mn + 2m + 2n) - \frac{1}{198mn + 2m + 2n}\Bigg[\log[2(m+n)(3)^{(3)}] \\
&\quad + \log[(3mn - m - n)(4)^{(4)}] + \log[(30mn)(5)^{(5)}] + \log[(6mn)(6)^{(6)}]\Bigg].
\end{aligned}
$$

- **The Second Zagreb Entropy of** $g - C_3N_5$
  From the definition of Second Zagreb index and edge partition, we get $M_2(G) = 228mn$. Applying the Second Zagreb entropy equation, we get the following result as

$$
\begin{aligned}
ENT_{M_2(G)} &= \log(M_2(G)) - \frac{1}{M_2(G)} \log\Bigg[\prod_{pq\in E_1} (d_p \times d_q)^{(d_p\times d_q)} \times \prod_{pq\in E_2} (d_p \times d_q)^{(d_p\times d_q)} \times \\
&\quad \prod_{pq\in E_3} (d_p \times d_q)^{(d_p\times d_q)} \times \prod_{pq\in E_4} (d_p \times d_q)^{(d_p\times d_q)}\Bigg] \\
&= \log(M_2(G)) - \frac{1}{M_2(G)} \log\Bigg[\Big(2(m+n)(2)^{(2)}\Big) \times \Big((3mn - m - n)(4)^{(4)}\Big) \times \Big((30mn)(6)^{(6)}\Big) \\
&\quad \times \Big((6mn)(9)^{(9)}\Big)\Bigg] \\
&= \log(228mn) - \frac{1}{228mn}\Bigg[\log[2(m+n)(2)^{(2)}] + \log[(3mn - m - n)(4)^{(4)}] + \log[(30mn)(6)^{(6)}] \\
&\quad + \log[(6mn)(9)^{(9)}]\Bigg].
\end{aligned}
$$

- **The Third Zagreb Entropy of** $g - C_3N_5$
  From the definition of Third Zagreb index and edge partition, we get $ZG_3(G) = 30mn + 2m + 2n$. Applying the third zagreb entropy equation, we get the following result as:

$$ENT_{ZG_3(G)} = \log(ZG_3(G)) - \frac{1}{ZG_3(G)} \log\Big[\prod_{12 \in E_1} |1-2|^{|1-2|} \times \prod_{(2,2) \in E_2} |2-2|^{|2-2|} \times$$
$$\prod_{(2,3) \in E_3} |2-3|^{|2-3|} \times \prod_{(3,3) \in E_4} |3-3|^{|3-3|} \Big]$$
$$= \log(ZG_3(G)) - \frac{1}{ZG_3(G)} \log\Bigg[\Big(2(m+n)(1)^{(1)} \Big)$$
$$\times \Big((3mn - m - n)(0)^{(0)} \Big) \times \Big((30mn)(1)^{(1)} \Big) \times \Big((6mn)(0)^{(0)} \Big) \Bigg]$$
$$= \log(30mn + 2m + 2n) - \frac{\log(2(m+n))}{30mn + 2m + 2n} - \frac{\log(30mn)}{30mn + 2m + 2n}.$$

- **The Atom-Bond Connectivity Entropy of** $g - C_3N_5$
  From the definition of Atom bond connectivity index and edge partition, we get:
  $ABC(G) = 29.334mn + 2.121m + 2.121n$.
  Applying the atom bond connectivity entropy equation, we get the following result as:

$$ENT_{ABC(G)} = \log(ABC(G)) - \frac{1}{ABC(G)} \log\Bigg[\prod_{pq \in E_1} \left(\sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}} \right) \times$$
$$\prod_{pq \in E_2} \left(\sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}} \right) \times \prod_{pq \in E_3} \left(\sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}} \right) \times \prod_{pq \in E_4} \left(\sqrt{\frac{d_p + d_q - 2}{d_p \cdot d_q}} \right) \Bigg]$$
$$= \log(29.334mn + 2.121m + 2.121n) - \frac{1}{29.334mn + 2.121m + 2.121n} \log\Bigg[\left(2(m+n) \left(\frac{1}{\sqrt{2}} \right)^{\left(\frac{1}{\sqrt{2}} \right)} \right)$$
$$\times \left((3mn - m - n) \left(\frac{1}{\sqrt{2}} \right)^{\left(\frac{1}{\sqrt{2}} \right)} \right) \times \left((30mn) \left(\frac{1}{\sqrt{2}} \right)^{\left(\frac{1}{\sqrt{2}} \right)} \right) \times \left((6mn) \left(\frac{2}{3} \right)^{\left(\frac{2}{3} \right)} \right) \Bigg]$$
$$= \log(29.334mn + 2.121m + 2.121n) - \frac{1}{29.334mn + 2.121m + 2.121n} \Bigg[\log \left(2(m+n) \left(\frac{1}{\sqrt{2}} \right)^{\left(\frac{1}{\sqrt{2}} \right)} \right)$$
$$+ \log\left((3mn - m - n) \left(\frac{1}{\sqrt{2}} \right)^{\left(\frac{1}{\sqrt{2}} \right)} \right) + \log\left((30mn) \left(\frac{1}{\sqrt{2}} \right)^{\left(\frac{1}{\sqrt{2}} \right)} \right) + \log\left((6mn) \left(\frac{2}{3} \right)^{\left(\frac{2}{3} \right)} \right) \Bigg].$$

- **The Geometric-Arithmetic Entropy of** $g - C_3N_5$
  From the definition of Geometric arithmetic index and edge partition, we get:
  $GA(G) = 38.393mn + 2.656m + 2.656n$.
  Applying the Geometric-arithmetic entropy equation, we get the following result as:

$$
\begin{aligned}
ENT_{GA(G)} &= \log(GA(G)) - \frac{1}{GA(G)} \log\Bigg[\prod_{pq \in E_1(G)} \left(\frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q} \right)^{\left(\frac{2\sqrt{d_p \cdot d_q}}{d_p+d_q}\right)} \times \\
&\prod_{pq \in E_2(G)} \left(\frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q} \right)^{\left(\frac{2\sqrt{d_p \cdot d_q}}{d_p+d_q}\right)} \times \prod_{pq \in E_3(G)} \left(\frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q} \right)^{\left(\frac{2\sqrt{d_p \cdot d_q}}{d_p+d_q}\right)} \times \prod_{pq \in E_4(G)} \left(\frac{2\sqrt{d_p \cdot d_q}}{d_p + d_q} \right)^{\left(\frac{2\sqrt{d_p \cdot d_q}}{d_p+d_q}\right)} \Bigg] \\
&= \log(38.393mn + 2.656m + 2.656n) - \frac{1}{38.393mn + 2.656m + 2.656n} \log\Bigg[\left(2(m+n) \left(\frac{2\sqrt{2}}{3} \right)^{\left(\frac{2\sqrt{2}}{3}\right)} \right) \\
&\times \Big((3mn - m - n) \Big) \times \left((30mn) \left(\frac{2\sqrt{6}}{5} \right)^{\left(\frac{2\sqrt{6}}{5}\right)} \right) \times (6mn) \Bigg] \\
&= \log(38.393mn + 2.656m + 2.656n) - \frac{1}{38.393mn + 2.656m + 2.656n} \Bigg[\log\left(2(m+n) \left(\frac{2\sqrt{2}}{3} \right)^{\left(\frac{2\sqrt{2}}{3}\right)} \right) \\
&- \log\Big((3mn - m - n) \Big) - \log\left((30mn) \left(\frac{2\sqrt{6}}{5} \right)^{\left(\frac{2\sqrt{6}}{5}\right)} \right) - \log(6mn) \Bigg].
\end{aligned}
$$

- **The Arithmetic-Geometric Entropy of** $g - C_3N_5$
  From the definition of Arithmetic-geometric index and edge partition, we get:
  $AG(G) = 39.618mn + 1.121m + 1.121n$.
  Applying the arithmetic geometric entropy equation, we get the following result as

$$
\begin{aligned}
ENT_{AG(G)} &= \log(AG(G)) - \frac{1}{AG(G)} \log\Bigg[\prod_{pq \in E_1(G)} \left(\frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}} \right)^{\left(\frac{d_p+d_q}{2\sqrt{d_p \cdot d_q}}\right)} \times \\
&\prod_{pq \in E_2(G)} \left(\frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}} \right)^{\left(\frac{d_p+d_q}{2\sqrt{d_p \cdot d_q}}\right)} \times \prod_{pq \in E_3(G)} \left(\frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}} \right)^{\left(\frac{d_p+d_q}{2\sqrt{d_p \cdot d_q}}\right)} \times \prod_{pq \in E_4(G)} \left(\frac{d_p + d_q}{2\sqrt{d_p \cdot d_q}} \right)^{\left(\frac{d_p+d_q}{2\sqrt{d_p \cdot d_q}}\right)} \Bigg] \\
&= \log(39.618mn + 1.121m + 1.121n) - \frac{1}{39.618mn + 1.121m + 1.121n} \log\Bigg[\left(2(m+n) \left(\frac{3}{2\sqrt{2}} \right)^{\left(\frac{3}{2\sqrt{2}}\right)} \right) \\
&\times \Big((3mn - m - n) \Big) \times \left((30mn) \left(\frac{5}{2\sqrt{6}} \right)^{\left(\frac{5}{2\sqrt{6}}\right)} \right) \times (6mn) \Bigg] \\
&= \log(39.618mn + 1.121m + 1.121n) - \frac{1}{39.618mn + 1.121m + 1.121n} \Bigg[\log\left(2(m+n) \left(\frac{3}{2\sqrt{2}} \right)^{\left(\frac{3}{2\sqrt{2}}\right)} \right) \\
&+ \log(3mn - m - n) + \log\left((30mn) \left(\frac{5}{2\sqrt{6}} \right)^{\left(\frac{5}{2\sqrt{6}}\right)} \right) + \log(6mn) \Bigg].
\end{aligned}
$$

- **The Harmonic Entropy of $g-C_3N_5$**
  From the definition of Harmonic index and edge partition, we get:
  $H(G) = 15.5mn + 0.833m + 0.833n$.
  Applying the Harmonic entropy equation we get the following result as:

$$
\begin{aligned}
ENT_{H(G)} &= \log(H(G)) - \frac{1}{H(G)} \log\Bigg[\prod_{pq\in E_1(G)} \left(\frac{2}{d_p+d_q}\right)^{\left(\frac{2}{d_p+d_q}\right)} \times \prod_{pq\in E_2(G)} \left(\frac{2}{d_p+d_q}\right)^{\left(\frac{2}{d_p+d_q}\right)} \times \\
&\prod_{pq\in E_3(G)} \left(\frac{2}{d_p+d_q}\right)^{\left(\frac{2}{d_p+d_q}\right)} \times \prod_{pq\in E_4(G)} \left(\frac{2}{d_p+d_q}\right)^{\left(\frac{2}{d_p+d_q}\right)}\Bigg] \\
&= \log(15.5mn + 0.833m + 0.833n) - \frac{1}{15.5mn + 0.833m + 0.833n} \log\Bigg[\left(2(m+n)\left(\frac{2}{3}\right)^{\left(\frac{2}{3}\right)}\right) \\
&\times \left((3mn-m-n)\left(\frac{1}{2}\right)^{\left(\frac{1}{2}\right)}\right) \times \left((30mn)\left(\frac{2}{5}\right)^{\left(\frac{2}{5}\right)}\right) \times \left((6mn)\left(\frac{2}{6}\right)^{\left(\frac{2}{6}\right)}\right)\Bigg] \\
&= \log(15.5mn + 0.833m + 0.833n) - \frac{1}{15.5mn + 0.833m + 0.833n} \Bigg[\log\left(2(m+n)\left(\frac{2}{3}\right)^{\left(\frac{2}{3}\right)}\right) \\
&+ \log\left((3mn-m-n)\left(\frac{1}{2}\right)^{\left(\frac{1}{2}\right)}\right) + \log\left((30mn)\left(\frac{2}{5}\right)^{\left(\frac{2}{5}\right)}\right) + \log\left((6mn)\left(\frac{2}{6}\right)^{\left(\frac{2}{6}\right)}\right)\Bigg].
\end{aligned}
$$

- **The Forgotten Entropy of $g-C_3N_5$**
  From the definition of Forgotten index and edge partition, we get:
  $F(G) = 522mn + 2m + 2n$.
  Applying the Forgotten entropy equation, we get the following result as:

$$
\begin{aligned}
ENT_{F(G)} &= \log(F(G)) - \frac{1}{F(G)} \log\Bigg[\prod_{pq\in E_1(G)} ({d_p}^2+{d_q}^2)^{\left({d_p}^2+{d_q}^2\right)} \times \prod_{pq\in E_2(G)} ({d_p}^2+{d_q}^2)^{\left({d_p}^2+{d_q}^2\right)} \times \\
&\prod_{pq\in E_3(G)} ({d_p}^2+{d_q}^2)^{\left[{d_p}^2+{d_q}^2\right]} \times \prod_{pq\in E_4(G)} ({d_p}^2+{d_q}^2)^{\left({d_p}^2+{d_q}^2\right)}\Bigg] \\
&= \log(522mn + 2m + 2n) - \frac{1}{522mn + 2m + 2n} \log\Bigg[\Big((2(m+n)(2)^{(2)}\Big) \\
&\times \Big((3mn-m-n)(4)^{(4)}\Big) \times \Big((30mn)(6)^{(6)}\Big) \times \Big((6mn)(9)^{(9)}\Big)\Bigg] \\
&= \log(522mn + 2m + 2n) - \frac{1}{522mn + 2m + 2n} \Bigg[\log(2(m+n)(2)^{(2)}) + \log((3mn-m-n)(4)^{(4)}) \\
&+ \log((30mn)(6)^{(6)}) + \log((6mn)(9)^{(9)})\Bigg].
\end{aligned}
$$

- **The Randić Entropy of $g-C_3N_5$ for $\alpha = 1$**
  From the definition of Randić entropy for $\alpha = 1$ and edge partition, we get:
  $R_1(G) = 228mn$.

Applying the Randić entropy equation, we get the following result as:

$$ENT_{R_1} = \log(R_1) - \frac{1}{R_1}\log\Big[\prod_{pq\in E_1}(d_p\times d_q)^{(d_p\times d_q)}\times\prod_{pq\in E_2}(d_p\times d_q)^{(d_p\times d_q)}$$
$$\times\prod_{pq\in E_3}(d_p\times d_q)^{(d_p\times d_q)}\times\prod_{pq\in E_4}(d_p\times d_q)^{(d_p\times d_q)}\Big]$$
$$=\log(228mn)-\frac{1}{228mn}\log\Big[\Big(2(m+n)(2)^2\Big)\times\Big((3mn-m-n)(4)^{(4)}\Big)\times\big((30mn)(6)^6\big)\times$$
$$\Big((6mn)(9)^{(9)}\Big)\Big]$$
$$=\log(228mn)-\frac{1}{228mn}\Big[\log\Big(2(m+n)(2)^{(2)}\Big)+\log\Big((3mn-m-n)(4)^{(4)}\Big)+\log\big((30mn)(6)^6\big)$$
$$+\log\Big((6mn)(3)^{(3)}\Big)\Big].$$

- **The Randić Entropy of $g-C_3N_5$ for $\alpha=\frac{1}{2}$**
From the definition of Randić entropy for $\alpha=\frac{1}{2}$ and edge partition, we get:
$R_{\frac{1}{2}}(G)=97.484mn+0.828m+0.828n.$
Applying the Randić entropy equation, we get the following result as:

$$ENT_{R_{\frac{1}{2}}} = \log(R_{\frac{1}{2}}) - \frac{1}{R_{\frac{1}{2}}}\log\Big[\prod_{pq\in E_1}\Big(\sqrt{d_p\times d_q}\Big)^{(\sqrt{d_p\times d_q})}\times\prod_{pq\in E_2}\Big(\sqrt{d_p\times d_q}\Big)^{(\sqrt{d_p\times d_q})}$$
$$\times\prod_{pq\in E_3}\Big(\sqrt{d_p\times d_q}\Big)^{(\sqrt{d_p\times d_q})}\times\prod_{pq\in E_4}\Big(\sqrt{d_p\times d_q}\Big)^{(\sqrt{d_p\times d_q})}\Big]$$
$$=\log(97.484mn+0.828m+0.828n)-\frac{1}{97.484mn+0.828m+0.828n}\log\Big[\Big(2(m+n)(\sqrt{2})^{\sqrt{2}}\Big)$$
$$\times\Big((3mn-m-n)(2)^{(2)}\Big)\times\Big((30mn)(\sqrt{6})^{\sqrt{6}}\Big)\times\Big((6mn)(3)^{(3)}\Big)\Big]$$
$$=\log(97.484mn+0.828m+0.828n)-\frac{1}{97.484mn+0.828m+0.828n}\Big[\log\Big(2(m+n)(\sqrt{2})^{\sqrt{(2)}}\Big)$$
$$+\log\Big((3mn-m-n)(2)^{(2)}\Big)+\log\Big((30mn)(\sqrt{6})^{\sqrt{6}}\Big)+\log\Big((6mn)(3)^{(3)}\Big)\Big].$$

- **The Randić Entropy of $g-C_3N_5$ for $\alpha=\frac{-1}{2}$**
From the definition of Randić entropy for $\alpha=\frac{-1}{2}$ and edge partition, we get:
$R_{\frac{-1}{2}}(G)=11.747mn+1.914m+1.914n.$

Applying the Randić entropy equation, we get the following result as:

$$ENT_{R_{\frac{-1}{2}}} = \log(R_{\frac{-1}{2}}) - \frac{1}{R_{\frac{-1}{2}}} \log\Big[\prod_{pq\in E_1}\left(\frac{1}{\sqrt{d_p\times d_q}}\right)^{\left(\frac{1}{\sqrt{d_p\times d_q}}\right)} \times \prod_{pq\in E_2}\left(\frac{1}{\sqrt{d_p\times d_q}}\right)^{\left(\frac{1}{\sqrt{d_p\times d_q}}\right)} \times$$

$$\prod_{pq\in E_3}\left(\frac{1}{\sqrt{d_p\times d_q}}\right)^{\left(\frac{1}{\sqrt{d_p\times d_q}}\right)} \times \prod_{pq\in E_4}\left(\frac{1}{\sqrt{d_p\times d_q}}\right)^{\left(\frac{1}{\sqrt{d_p\times d_q}}\right)}\Big]$$

$$= \log(11.747mn + 1.914m + 1.914n) - \frac{1}{11.747mn + 1.914m + 1.914n} \log\Bigg[\left(2(m+n)\left(\frac{1}{\sqrt{2}}\right)^{\left(\frac{1}{\sqrt{2}}\right)}\right)$$

$$\times \left((3mn - m - n)\left(\frac{1}{2}\right)^{\left(\frac{1}{2}\right)}\right) \times \left((30mn)\left(\frac{1}{\sqrt{6}}\right)^{\left(\frac{1}{\sqrt{6}}\right)}\right) \times \left((6mn)\left(\frac{1}{3}\right)^{\left(\frac{1}{3}\right)}\right)\Bigg]$$

$$= \log(11.747mn + 1.914m + 1.914n) - \frac{1}{11.747mn + 1.914m + 1.914n} \log\Bigg[\left(2(m+n)\left(\frac{1}{\sqrt{2}}\right)^{\left(\frac{1}{\sqrt{2}}\right)}\right)$$

$$+ \log\left((3mn - m - n)\left(\frac{1}{2}\right)^{\left(\frac{1}{2}\right)}\right) + \log\left((30mn)\left(\frac{1}{\sqrt{6}}\right)^{\left(\frac{1}{\sqrt{6}}\right)}\right) + \log\left((6mn)\left(\frac{1}{3}\right)^{\left(\frac{1}{3}\right)}\right)\Bigg].$$

- **The Randić Entropy of $g - C_3N_5$ for $alpha = -1$**
  From the definition of Randić entropy for $\alpha = -1$ and edge partition, we get:
  $R_{-1}(G) = 6.416mn + 0.75m + 0.75n$.
  Applying the Randić entropy equation, we get the following result as:

$$ENT_{R_{-1}} = \log(R_{-1}) - \frac{1}{R_{-1}} \log\Big[\prod_{pq\in E_1}\left(\frac{1}{d_p\times d_q}\right)^{\left(\frac{1}{d_p\times d_q}\right)} \times \prod_{pq\in E_2}\left(\frac{1}{d_p\times d_q}\right)^{\left(\frac{1}{d_p\times d_q}\right)} \times$$

$$\prod_{pq\in E_3}\left(\frac{1}{d_p\times d_q}\right)^{\left(\frac{1}{d_p\times d_q}\right)} \times \prod_{pq\in E_4}\left(\frac{1}{d_p\times d_q}\right)^{\left(\frac{1}{d_p\times d_q}\right)}\Big]$$

$$= \log(6.416mn + 0.75m + 0.75n) - \frac{1}{6.416mn + 0.75m + 0.75n} \log\Bigg[\left(2(m+n)\left(\frac{1}{2}\right)^{\left(\frac{1}{2}\right)}\right)$$

$$\times \left((3mn - m - n)\left(\frac{1}{4}\right)^{\left(\frac{1}{4}\right)}\right) \times \left((30mn)\left(\frac{1}{6}\right)^{\left(\frac{1}{6}\right)}\right) \times \left((6mn)\left(\frac{1}{9}\right)^{\left(\frac{1}{9}\right)}\right)\Bigg]$$

$$= \log(6.416mn + 0.75m + 0.75n) - \frac{1}{6.416mn + 0.75m + 0.75n} \Bigg[\log\left(2(m+n)\left(\frac{1}{2}\right)^{\left(\frac{1}{2}\right)}\right)$$

$$+ \log\left((3mn - m - n)\left(\frac{1}{4}\right)^{\left(\frac{1}{4}\right)}\right) + \log\left((30mn)\left(\frac{1}{6}\right)^{\left(\frac{1}{6}\right)}\right) + \log\left((6mn)\left(\frac{1}{9}\right)^{\left(\frac{1}{9}\right)}\right)\Bigg].$$

5. Numerical Results and Discussions

Throughout this section, the numerical values of above degree-based entropy measures are determined by altering the value of the variable m and n from 1 to 10 in the analytical formulation of $g - C_3N_5$ structure. These values are presented in Tables 2-5. This activity is carried out to examine the numerical similarities and variations between individual topological indices. The computational findings demonstrated that degree-based entropy estimates are very sensitive to the value of m and n. The Figures 2-5 demonstrate that the entropy measures for each of the above topological indices derived in this work increase as m and n increase from 1 to 10. The measures expand researcher's possibilities to understand the physico- chemical relationships between the chemical structures according to the investigation.

Table 2: Numerical Comparison of entropies of First, Second and Third Zagreb indices.

[m,n]	[1,1]	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]	[8,8]	[9,9]	[10,10]
ENT_{M_1}	2.231	2.881	3.243	3.496	3.692	3.851	3.985	4.102	4.204	4.296
ENT_{M_2}	2.274	2.936	3.301	3.555	3.751	3.911	4.045	4.162	4.264	4.356
ENT_{ZG_3}	1.470	2.083	2.437	2.687	2.881	3.038	3.172	3.288	3.389	3.481

Table 3: Numerical Comparison of entropies of ABC, GA, AG

[m,n]	[1,1]	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]	[8,8]	[9,9]	[10,10]
ENT_{ABC}	1.369	2.064	2.398	2.674	2.986	3.015	3.142	3.276	3.378	3.469
ENT_{GA}	1.575	2.176	2.531	2.783	2.978	3.137	3.271	3.387	3.490	3.581
ENT_{AG}	1.552	2.179	2.542	2.796	2.992	3.152	3.286	3.403	3.505	3.597

Table 4: Numerical Comparison of Harmonic and Forgotten entropy

[m,n]	[1,1]	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]	[8,8]	[9,9]	[10,10]
ENT_H	1.102	1.743	2.118	2.378	2.578	2.740	2.875	2.993	3.096	3.188
ENT_F	2.624	3.296	3.661	3.916	4.111	4.271	4.406	4.522	4.625	4.716

Table 5: Numerical Comparison of $R_1(G)$, $R_{-1}(G)$, $R_{\frac{1}{2}}(G)$, $R_{\frac{-1}{2}}(G)$

[m,n]	[1,1]	[2,2]	[3,3]	[4,4]	[5,5]	[6,6]	[7,7]	[8,8]	[9,9]	[10,10]
ENT_{R_1}	2.274	2.936	3.301	3.555	3.751	3.911	4.045	4.162	4.264	4.356
$ENT_{R_{\frac{1}{2}}}$	1.939	2.574	2.935	3.188	3.383	3.543	3.677	3.794	3.896	3.988
$ENT_{R_{-1}}$	0.605	1.292	1.697	1.972	2.179	2.346	2.489	2.604	2.709	2.802
$ENT_{R_{\frac{-1}{2}}}$	1.045	1.651	2.017	2.274	2.471	2.630	2.765	2.881	2.984	3.075

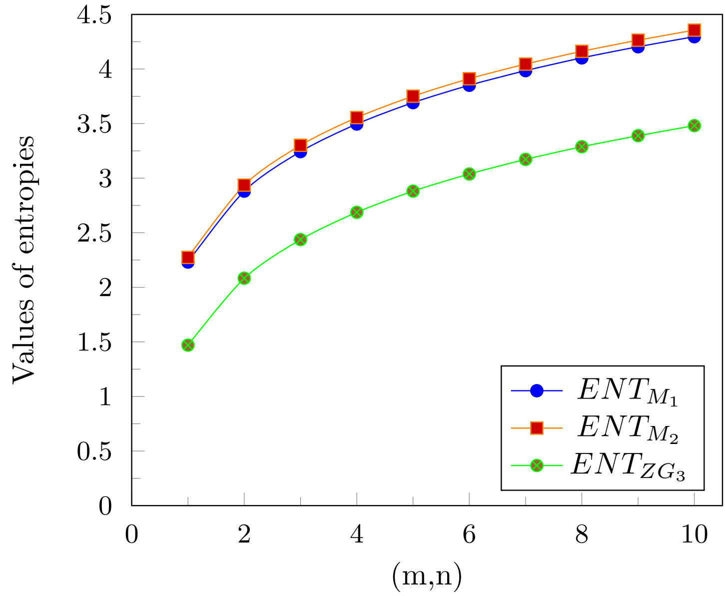

Figure 2: Comparision of ENT_{M_1}, ENT_{M_2} and ENT_{ZG_3} of $g - C_3N_5$

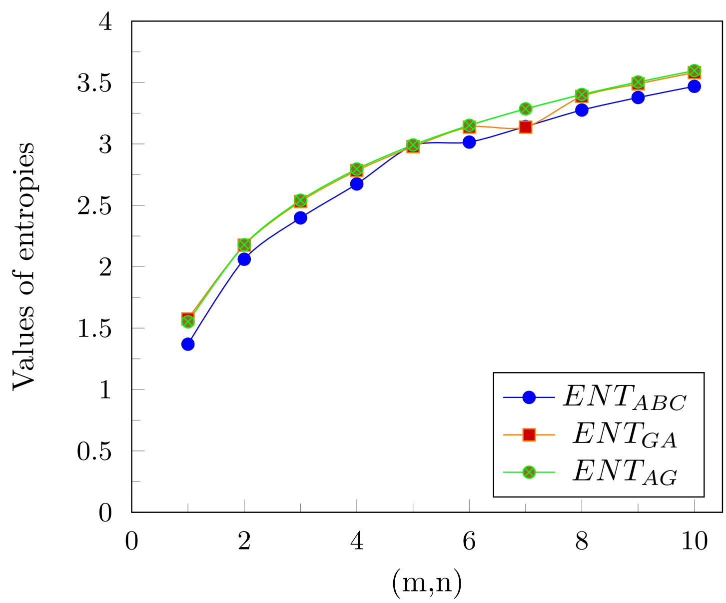

Figure 3: Comparision of ENT_{ABC}, ENT_{GA} and ENT_{AG} of $g - C_3N_5$

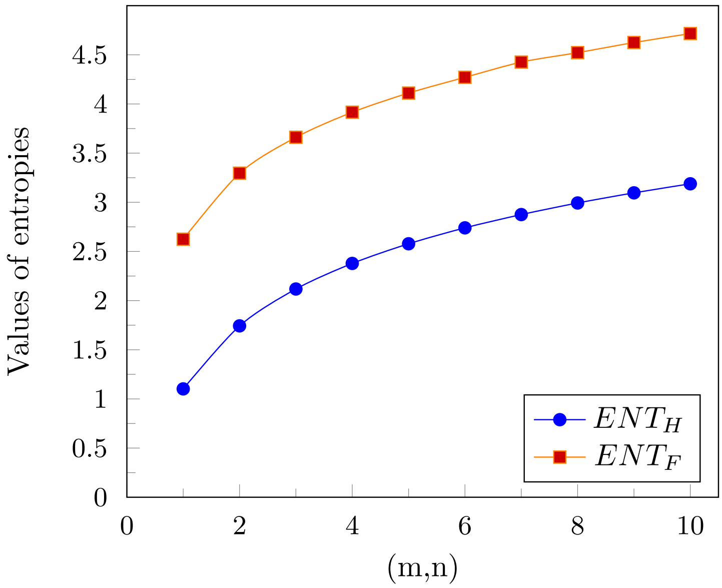

Figure 4: Comparision of ENT_H, ENT_F of $g - C_3N_5$

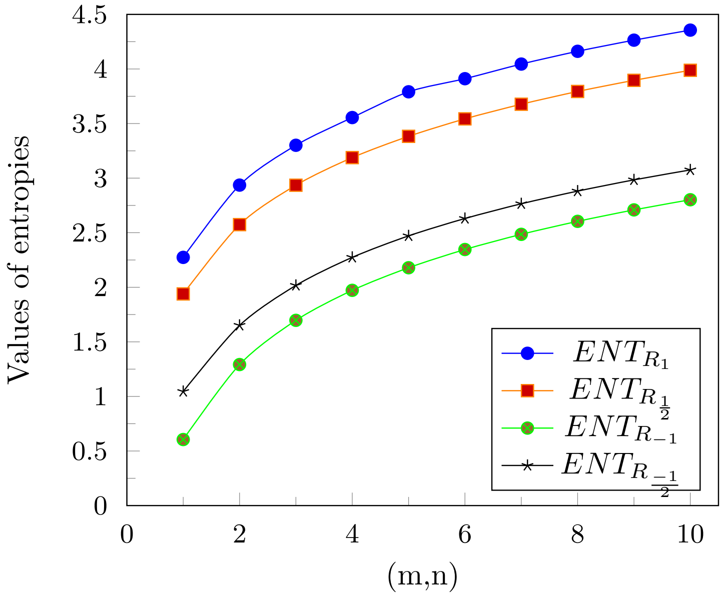

Figure 5: Comparision of ENT_{R_1}, $ENT_{R_{-1}}$, $ENT_{R_{\frac{1}{2}}}$, $ENT_{R_{\frac{-1}{2}}}$ of $g - C_3N_5$

6. Conclusion

In this work we explore the graph entropies associated with the new information function, based in shannon's definitions of entropy. we present a correspondence between degree based entropies and degree-based topological indices. We calculated the entropies based on degree for graphitic carbon nitride. The numerical values of these entropies allow us to compare degree-based entropies with degree-based topological indices, which aids in our understanding of the physico-chemical characteristics of the graphitic carbon nitride structure. We wish to expand this concept in the future to different chemical structures that investigate the researcher's new line of inquiry in this area.

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E. Lavanya
Department of Mathematics
Vidyavardhaka College of Engineering, Mysuru-570 002, India.
Affiliated to Visvesvaraya Technological University
Belagavi-590 018, India.
&
Department of Mathematics
Acharya Institute of Graduate Studies
Bengaluru-560 107, India.
E-mail address: lavanya.hup@gmail.com

and

M. A. Sriraj (Corresponding author)
Department of Mathematics
Vidyavardhaka College of Engineering, Mysuru-570 002, India.
Affiliated to Visvesvaraya Technological University
Belagavi-590 018, India.
E-mail address: masriraj@gmail.com

and

P. Siva Kota Reddy
Department of Mathematics
JSS Science and Technology University
Mysuru-570 006, India.
E-mail address: pskreddy@jssstuniv.in