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Research Paper

On Nirmala Indices–based Entropy Measures of Silicon Carbide Network

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Abstract

Topological indices are numerical parameters for understanding the fundamental topology of chemical structures that correlate with the quantitative structure-property relationship (QSPR) / quantitative structure-activity relationship (QSAR) of chemical compounds. The M-polynomial is a modern mathematical approach to finding the degree-based topological indices of molecular graphs. Several graph assets have been employed to discriminate the construction of entropy measures from the molecular graph of a chemical compound. Graph entropies have evolved as information-theoretic tools to investigate the structural information of a molecular graph. The possible applications of graph entropy measures in chemistry, biology and discrete mathematics have drawn the attention of researchers. In this research work, we compute the Nirmala index, first and second inverse Nirmala index for silicon carbide network Si_2C_3-$I[p,q]$ with the help of its M-polynomial. Further, we introduce the concept of Nirmala indices-based entropy measure and enumerate them for the above-said network. Additionally, the comparison and correlation between the Nirmala indices and their associated entropy measures are presented through numerical computation and graphical approaches. Following that, curve fitting and correlation analysis are performed to investigate the relationship between the Nirmala indices and corresponding entropy measures.

1 Introduction

Let $\Upsilon = (V(\Upsilon), E(\Upsilon))$ be an ordered pair of a simple, connected and undirected graph with non-empty vertex set $V(\Upsilon)$ and edge set $E(\Upsilon)$. The degree $d_\Upsilon(u)$ of a vertex $u \in V(\Upsilon)$ is the

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total number of edges incident to u. An edge of the graph Υ is denoted by $e = uv$ or vu, where u and v are end vertices of that edge [1].

A constitutive branch of mathematical chemistry that confluent mathematics and chemistry by employing the graph theory is known as chemical graph theory (CGT). In CGT, the molecular structure of a chemical compound is interpreted as a graph where the atoms and bonds of the molecular structure correspond to the vertices and edges of the graph, respectively. In this allied area of science, molecular structures are mathematically analyzed through theoretical, computational and graphical techniques [2].

Topological indices are mathematical parameters of a molecular graph associated with the chemical compound that is utilized to predict the physical characteristics, chemical properties, and biological activities of that compound. These indices play a significant role in the development of the quantitative structure-property relationship (QSPR) / quantitative structure-activity relationship (QSAR) analysis [3, 4]. Mathematically, a topological index is a function from the set of all simple, connected and undirected graphs to the set of real numbers which remain unchanged for isomorphic graphs.

As mentioned in [5], the degree-based topological index defined on edge set $E(\Upsilon)$ of a graph Υ can be denoted as:

$$I(\Upsilon) = \sum_{uv \in E(\Upsilon)} f(d_\Upsilon(u), d_\Upsilon(v)),$$

where $f(x, y)$ is a non-negative and symmetric function that depends on the mathematical formulation of the topological index. The above definition of the topological index can also be formulated as:

$$I(\Upsilon) = \sum_{i \leq j} m_{i,j}(\Upsilon) f(i, j),$$

where $m_{i,j}$ is the total number of edges $uv \in E(\Upsilon)$ such that $d_\Upsilon(u) = i$, $d_\Upsilon(v) = j$ $(i, j \geq 1)$.

In the literature, several topological indices have been introduced and have proven their usability in many areas of science and technology such as chemistry, mathematics, computer science, biology, drug discovery, etc. Wiener index is the first theoretically most investigated topological index. It was proposed by H. Wiener in 1947 and has significant application to predict the boiling points of paraffin [6]. The connectivity index (or Randić index) was proposed by Milan Randić in 1975. It is a very well-known degree-based topological index and has widespread application in drug discovery [7]. Other well-known degree-based topological indices that have substantiated their applicability are the Zagreb indices, harmonic index, symmetric division (deg) index, atom-bond connectivity index, geometric-arithmetic index, inverse sum (indeg) index and augmented Zagreb index, etc. For more details on the topological indices and their usability, researchers may follow the articles [4, 8–11] and their references cited therein.

Several initiatives have been attempted to improve the predictive potential of these indices by introducing a new index in the class of degree-based topological indices. Very recently, V.R. Kulli innovated a degree-based topological index namely the Nirmala index [12] of a molecular graph Υ, and described its mathematical formula as:

$$N(\Upsilon) = \sum_{uv \in E(\Upsilon)} \sqrt{d_\Upsilon(u) + d_\Upsilon(v)}. \tag{1}$$

Further, the first inverse Nirmala index (denoted as $IN_1(\Upsilon)$) and second inverse Nirmala index (denoted as $IN_2(\Upsilon)$) of a molecular graph Υ are established by Kulli et al. [13] in 2021 which are defined as follows:

$$IN_1(\Upsilon) = \sum_{uv \in E(\Upsilon)} \sqrt{\frac{1}{d_\Upsilon(u)} + \frac{1}{d_\Upsilon(v)}} = \sum_{uv \in E(\Upsilon)} \left[\frac{1}{d_\Upsilon(u)} + \frac{1}{d_\Upsilon(v)}\right]^{\frac{1}{2}}, \tag{2}$$

$$IN_2(\Upsilon) = \sum_{uv \in E(\Upsilon)} \frac{1}{\sqrt{\frac{1}{d_\Upsilon(u)} + \frac{1}{d_\Upsilon(v)}}} = \sum_{uv \in E(\Upsilon)} \left[\frac{1}{d_\Upsilon(u)} + \frac{1}{d_\Upsilon(v)}\right]^{-\frac{1}{2}}. \quad (3)$$

In the past, several topological indices were calculated using their standard mathematical definition. Multiple attempts are made to investigate a compact approach that can recover numerous topological indices of a certain class. In this connection, the idea of a general polynomial was established whose derivatives or integrals, or a mix of both, at a particular point produce the values of required topological indices. For example, the Hosoya polynomial [14] is utilized to recover the distance-based topological indices and NM-polynomial [15] produces the neighborhood degree sum-based indices. In 2015, Deutsch and Klažar proposed the concept of the M-polynomial [16] to deal with the computation of degree-based topological indices. In [17–22], several degree-based topological indices are calculated using the M-polynomial.

Definition 1.1 ([16])**.** The M-polynomial of a graph Υ defined as:

$$M(\Upsilon; x, y) = \sum_{\delta \le i \le j \le \Delta} m_{i,j}(\Upsilon)\ x^i y^j,$$

where $\delta = \min\{d_\Upsilon(u) | u \in V(\Upsilon)\}$, $\Delta = \max\{d_\Upsilon(u) | u \in V(\Upsilon)\}$ and $m_{i,j}(\Upsilon)$ is the number of edges $uv \in E(\Upsilon)$ such that $d_\Upsilon(u) = i$, $d_\Upsilon(v) = j$ $(i, j \ge 1)$.

Now, we list the M-polynomial-based derivation formulas to compute the different Nirmala indices in Table 1.

Table 1: Relation of the Nirmala indices with M-polynomial [23] of a graph Υ.

S. No.	**Topological Index**	**f(x,y)**	**Derivation from $M(\Upsilon; x, y)$**
1.	Nirmala index (N)	$\sqrt{x+y}$	$D_x^{1/2} J[M(\Upsilon; x, y)]\|_{x=1}$
2.	First inverse Nirmala index (IN_1)	$\sqrt{\frac{x+y}{xy}}$	$D_x^{1/2} J S_y^{1/2} S_x^{1/2}[M(\Upsilon; x, y)]\|_{x=1}$
3.	Second inverse Nirmala index (IN_2)	$\sqrt{\frac{xy}{x+y}}$	$S_x^{1/2} J D_y^{1/2} D_x^{1/2}[M(\Upsilon; x, y)]\|_{x=1}$

The operators $D_x^{1/2}$, $D_y^{1/2}$, $S_x^{1/2}$, $S_y^{1/2}$, and J mentioned in Table 1 are defined as follows:

$$D_x^{1/2}(h(x,y)) = \sqrt{x \frac{\partial(h(x,y))}{\partial x}}.\sqrt{h(x,y)}, \qquad D_y^{1/2}(h(x,y)) = \sqrt{y \frac{\partial(h(x,y))}{\partial y}}.\sqrt{h(x,y)},$$

$$S_x^{1/2}(h(x,y)) = \sqrt{\int_0^x \frac{h(t,y)}{t} dt}.\sqrt{h(x,y)}, \qquad S_y^{1/2}(h(x,y)) = \sqrt{\int_0^y \frac{h(x,t)}{t} dt}.\sqrt{h(x,y)},$$

$$J(h(x,y)) = h(x,x).$$

Shannon proposed the primary concept of entropy [24] in 1948 and stated that a measure of the uncertainty of a system or a measure of the unpredictability of information content is called the entropy of a probability distribution. Hereafter, entropy was commenced to be enforced on chemical structures or networks and graphs to analyze their structural information. In recent times, the applications of graph entropies have grown significantly across a wide range of disciplines, including computer science, mathematics, biology, chemistry, sociology, and ecology.

Graph entropy measures can be classified into different types such as intrinsic and extrinsic measures, and they correspond to the probability distribution with graph invariants (edges, vertices, etc.). More details on degree-based graph entropy measures and their applications can be seen in references [25–28].

1.1 Entropy of a graph in terms of vertex degree

Let us consider the above-defined simple and connected graph Υ with order n and size m. Then, the graph entropy [24], introduced by Shannon, of a graph Υ is defined as follows:

$$ENT_{\omega}(\Upsilon) = -\sum_{i=1}^{n} \frac{\omega(s_i)}{\sum_{j=1}^{n} \omega(s_j)} \log\left(\frac{\omega(s_i)}{\sum_{j=1}^{n} \omega(s_j)}\right), \tag{4}$$

where ω is a meaningful information function and $s_i \in V(\Upsilon)$ for each $i \in \{1, 2, 3 \dots n\}$.
Now, consider $\omega(s_i) = d_{\Upsilon}(s_i)$ then Equation (4) reduces to

$$ENT_{\omega}(\Upsilon) = -\sum_{i=1}^{n} \frac{d_{\Upsilon}(s_i)}{\sum_{j=1}^{n} d_{\Upsilon}(s_j)} \log\left(\frac{d_{\Upsilon}(s_i)}{\sum_{j=1}^{n} d_{\Upsilon}(s_j)}\right),$$

thus

$$ENT_{\omega}(\Upsilon) = \log\left(\sum_{j=1}^{n} d_{\Upsilon}(s_j)\right) - \frac{1}{(\sum_{j=1}^{n} d_{\Upsilon}(s_j))} \sum_{i=1}^{n} d_{\Upsilon}(s_i) \log\left(d_{\Upsilon}(s_i)\right).$$

Since $\sum_{i=1}^{n} d_{\Upsilon}(s_i) = 2m$ (fundamental theorem of graph theory), the above equation becomes

$$ENT_{\omega}(\Upsilon) = \log(2m) - \frac{1}{2m} \sum_{i=1}^{n} d_{\Upsilon}(s_i) \log\left(d_{\Upsilon}(s_i)\right). \tag{5}$$

1.2 Entropy of a graph in terms of edge-weight

The concept of entropy [29] of an edge-weight graph is proposed by Chen et al. in 2014. Suppose Υ be an edge-weight graph represented as $\Upsilon = (V(\Upsilon), E(\Upsilon), \omega(st))$, where $V(\Upsilon)$ is a set of vertices, $E(\Upsilon)$ is a set of edges and $\omega(st)$ denotes the weight of an edge $st \in E(\Upsilon)$. Then the entropy of a graph in terms of edge-weight is defined as follows:

$$ENT_{\omega}(\Upsilon) = -\sum_{s't' \in E(\Upsilon)} \frac{\omega(s't')}{\sum_{st \in E(\Upsilon)} \omega(st)} \log\left(\frac{\omega(s't')}{\sum_{st \in E(\Upsilon)} \omega(st)}\right). \tag{6}$$

Equation (6) reduces to Equation (7) using the following steps

$$ENT_{\omega}(\Upsilon) = -\sum_{s't' \in E(\Upsilon)} \frac{\omega(s't')}{\sum_{st \in E(\Upsilon)} \omega(st)} \left[\log\left(\omega(s't')\right) - \log\left(\sum_{st \in E(\Upsilon)} \omega(st)\right)\right],$$

thus

$$ENT_{\omega}(\Upsilon) = \log\left(\sum_{st \in E(\Upsilon)} \omega(st)\right) - \sum_{s't' \in E(\Upsilon)} \frac{\omega(s't')}{\sum_{st \in E(\Upsilon)} \omega(st)} \log\left(\omega(s't')\right),$$

so

$$ENT_{\omega}(\Upsilon) = \log\Big(\sum_{st\in E(\Upsilon)} \omega(st)\Big) - \frac{1}{\Big(\sum_{st\in E(\Upsilon)} \omega(st)\Big)} \sum_{s't'\in E(\Upsilon)} \omega(s't') \log\left(\omega(s't')\right). \tag{7}$$

Now we introduce the Nirmala indices-based entropy by considering the meaningful information function ω as a function associated with the definitions of the Nirmala indices.

- **Nirmala entropy**

Let $\omega(st) = \sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)}$ then according to the definition of the Nirmala index as given in Equation (1), we have

$$\sum_{st\in E(\Upsilon)} \omega(st) = \sum_{st\in E(\Upsilon)} \sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)} = N(\Upsilon).$$

Now, Equation (7) leads to the following mathematical expression and is called the Nirmala entropy of a graph Υ. It is denoted as follows:

$$ENT_N(\Upsilon) = \log(N(\Upsilon)) - \frac{1}{N(\Upsilon)} \sum_{st\in E(\Upsilon)} \sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)} \times \log\Big(\sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)}\Big). \tag{8}$$

- **First inverse Nirmala entropy**

Let $\omega(st) = \sqrt{\frac{1}{d_{\Upsilon}(s)} + \frac{1}{d_{\Upsilon}(t)}}$ then as per the expression of the First inverse Nirmala index which is mentioned in Equation (2), we obtain

$$\sum_{st\in E(\Upsilon)} \omega(st) = \sum_{st\in E(\Upsilon)} \sqrt{\frac{1}{d_{\Upsilon}(s)} + \frac{1}{d_{\Upsilon}(t)}} = IN_1(\Upsilon).$$

Next, Equation (7) changes to the following expression and is called the first inverse Nirmala entropy of a graph Υ. It is defined as follows:

$$ENT_{IN_1}(\Upsilon) = \log(IN_1(\Upsilon)) - \frac{1}{IN_1(\Upsilon)} \sum_{st\in E(\Upsilon)} \sqrt{\frac{1}{d_{\Upsilon}(s)} + \frac{1}{d_{\Upsilon}(t)}} \times \log\left(\sqrt{\frac{1}{d_{\Upsilon}(s)} + \frac{1}{d_{\Upsilon}(t)}}\right). \tag{9}$$

- **Second inverse Nirmala entropy**

Let $\omega(st) = \frac{\sqrt{d_{\Upsilon}(s)d_{\Upsilon}(t)}}{\sqrt{d_{\Upsilon}(s)+d_{\Upsilon}(t)}}$ then employing the definition of the second inverse Nirmala index as defined in Equation (3), we get

$$\sum_{st\in E(\Upsilon)} \omega(st) = \sum_{st\in E(\Upsilon)} \frac{\sqrt{d_{\Upsilon}(s)d_{\Upsilon}(t)}}{\sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)}} = IN_2(\Upsilon).$$

Further, Equation (7) reduces to the following mathematical form and is called the second inverse Nirmala entropy of a graph Υ. It is denoted and defined as follows:

$$ENT_{IN_2}(\Upsilon) = \log(IN_2(\Upsilon)) - \frac{1}{IN_2(\Upsilon)} \sum_{st\in E(\Upsilon)} \frac{\sqrt{d_{\Upsilon}(s)d_{\Upsilon}(t)}}{\sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)}} \times \log\left(\frac{\sqrt{d_{\Upsilon}(s)d_{\Upsilon}(t)}}{\sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)}}\right). \tag{10}$$

1.3 Methodology and directions

In this paper, we introduce the concept of graph entropy measures by using new information functions based on the definitions of the different Nirmala indices and perform their mathematical and computational investigation for the silicon carbide network Si_2C_3-$I[p,q]$. Section 2 initiates with some basic preliminaries and a discussion of the $2D$ structure of the Si_2C_3-$I[p,q]$ network. Hereafter, we present the computation of the Nirmala indices using the M-polynomial to calculate the Nirmala indices-based entropy measures of the Si_2C_3-$I[p,q]$ network. Furthermore, the comparison of the Nirmala indices and their allied entropy measures is presented through numerical data, surface plots and $3D$ line plots in Section 3. In Section 4, we establish the best-fit regression models between the Nirmala indices and associated entropies using the curve-fitting tool in MATLAB R2019a software and execute the correlation analysis among all the molecular descriptors to observe their correlation with each other. At last, we conclude in Section 5.

2 Computation for silicon carbide network

Silicon carbide is an industrial, synthetic, and ceramic material. It is a non-toxic and inexpensive compound with innumerable assets. Hardness, robust crystal structure, high-temperature resistance, conductivity, and chemical stability are significant properties of silicon carbide, therefore it is used as a semiconductor in most technological devices like cutting-edge electronic gadgets, electric vehicles, solar power inverters, sensor systems, etc. To know more about its purification, development, and applications, see [30–32].

2.1 $2D$ Structure of Si_2C_3-*I[p,q]*

For the silicon carbide Si_2C_3-$I[p,q]$ network, the minimal energy of the Si_2C_3-I sheet exhibits a planner framework consisting of polygon rings where each hexagonal ring is surrounded by two pentagonal and four heptagonal rings. In the crystallographic structure of silicon carbide Si_2C_3-$I[p,q]$, p represents the number of associated unit cells in a single row and q represents the number of associated rows each with p number of cells. The $2D$ molecular graph of silicon carbide Si_2C_3-$I[p,q]$ is given in Figure 1 where we have demonstrated how the cells are associated in a row and how one row is associated with another row. Observe that, in the graph of Si_2C_3-$I[p,q]$, the total number of vertices is $10pq$ and the number of edges is $15pq - 2p - 3q$. Vertex set and edge set partitions of Si_2C_3-$I[p,q]$ are given in Tables 2 and 3, respectively.

Table 2: Vertex set partition of $\Upsilon = Si_2C_3$-$I[p,q]$ according to degrees of each vertex.

Vertex set	$d_\Upsilon(s)$	Total count
V_1	1	2
V_2	2	$4p + 6q - 4$
V_3	3	$10pq - 4p - 6q + 2$

2.2 Nirmala indices of Si_2C_3-*I[p,q]*

In [21], the M-polynomial of silicon carbide network Si_2C_3-$I[p,q]$ was obtained and it is given by the following theorem.

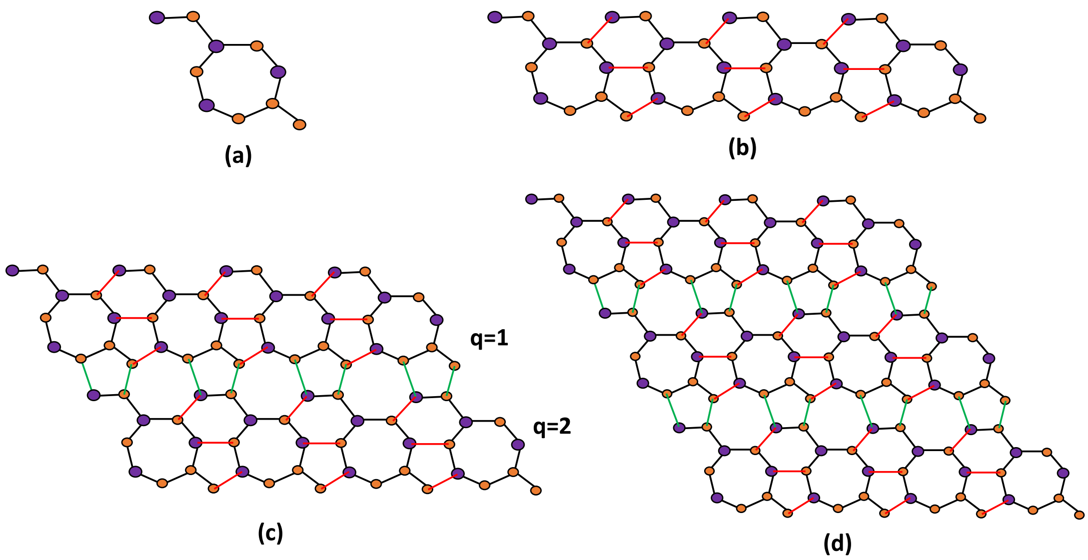


Figure 1: (a) Unit cell of Si_2C_3-$I[p,q]$, (b) Si_2C_3-$I[4,1]$, (c) Si_2C_3-$I[4,2]$, and (d) Si_2C_3-$I[4,3]$.

Table 3: Edge set partition of $\Upsilon = Si_2C_3$-$I[p,q]$ according to degrees of end vertices of an edge.

Edge set	$(d_\Upsilon(s), d_\Upsilon(t))$	**Total count**
E_1	$(1,2)$	1
E_2	$(1,3)$	1
E_3	$(2,2)$	$p+2q$
E_4	$(2,3)$	$6p+8q-9$
E_5	$(3,3)$	$15pq-9p-13q+7$

Theorem 2.1 ([21], Theorem 2.1)**.** *Let Υ be the silicon carbide Si_2C_3-$I[p,q]$. Then the M-polynomial of Υ is*

$$M(\Upsilon;x,y) = xy^2 + xy^3 + (p+2q)x^2y^2 + (6p+8q-9)x^2y^3 + (15pq-9p-13q+7)x^3y^3.$$

Now we evaluate the Nirmala indices of Si_2C_3-$I[p,q]$ with the help of its M-polynomial.

Theorem 2.2. *Let Υ be the silicon carbide network Si_2C_3-$I[p,q]$, then the Nirmala indices of Υ are*

(i) $N(\Upsilon) = 15\sqrt{6}pq + (2+6\sqrt{5}-9\sqrt{6})p + (4+8\sqrt{5}-13\sqrt{6})q + (2+\sqrt{3}-9\sqrt{5}+7\sqrt{6})$,

(ii) $IN_1(\Upsilon) = 5\sqrt{6}pq + (1+\sqrt{30}-3\sqrt{6})p + \big(2+\frac{8\sqrt{5}}{\sqrt{6}}-\frac{13\sqrt{6}}{3}\big)q + \big(\frac{\sqrt{3}}{\sqrt{2}}+\frac{2}{\sqrt{3}}-\frac{9\sqrt{5}}{\sqrt{6}}+\frac{7\sqrt{6}}{3}\big)$,

(iii) $IN_2(\Upsilon) = \frac{15\sqrt{3}}{\sqrt{2}}pq + \big(1+\frac{6\sqrt{6}}{\sqrt{5}}-\frac{9\sqrt{3}}{\sqrt{2}}\big)p + \big(2+\frac{8\sqrt{6}}{\sqrt{5}}-\frac{13\sqrt{3}}{\sqrt{2}}\big)q + \big(\frac{\sqrt{2}}{\sqrt{3}}+\frac{\sqrt{3}}{2}-\frac{9\sqrt{6}}{\sqrt{5}}+\frac{7\sqrt{3}}{\sqrt{2}}\big)$.

Proof. Let us now determine the derivation formulas (as mentioned in Table 1) over the M-polynomial $M(\Upsilon;x,y)$ at the point (x,y) to get the expressions of the Nirmala indices of Υ.

- $D_x^{1/2}J[M(\Upsilon;x,y)]$
$= D_x^{1/2}J[xy^2 + xy^3 + (p+2q)x^2y^2 + (6p+8q-9)x^2y^3 + (15pq-9p-13q+7)x^3y^3]$
$= D_x^{1/2}[x^3 + x^4 + (p+2q)x^4 + (6p+8q-9)x^5 + (15pq-9p-13q+7)x^6]$
$= \sqrt{3}x^3 + 2(p+2q+1)x^4 + \sqrt{5}(6p+8q-9)x^5 + \sqrt{6}(15pq-9p-13q+7)x^6,$

- $D_x^{1/2}JS_y^{1/2}S_x^{1/2}[M(\Upsilon;x,y)]$
$= D_x^{1/2}JS_y^{1/2}S_x^{1/2}[xy^2 + xy^3 + (p+2q)x^2y^2 + (6p+8q-9)x^2y^3 + (15pq-9p-13q+7)x^3y^3]$
$= D_x^{1/2}JS_y^{1/2}[xy^2 + xy^3 + \frac{1}{\sqrt{2}}(p+2q)x^2y^2 + \frac{1}{\sqrt{2}}(6p+8q-9)x^2y^3 + \frac{1}{\sqrt{3}}(15pq-9p-13q+7)x^3y^3]$
$= D_x^{1/2}J[\frac{1}{\sqrt{2}}xy^2 + \frac{1}{\sqrt{3}}xy^3 + \frac{1}{2}(p+2q)x^2y^2 + \frac{1}{\sqrt{6}}(6p+8q-9)x^2y^3 + \frac{1}{3}(15pq-9p-13q+7)x^3y^3]$
$= D_x^{1/2}[\frac{1}{\sqrt{2}}x^3 + \frac{1}{\sqrt{3}}x^4 + \frac{1}{2}(p+2q)x^4 + \frac{1}{\sqrt{6}}(6p+8q-9)x^5 + \frac{1}{3}(15pq-9p-13q+7)x^6]$
$= \frac{\sqrt{3}}{\sqrt{2}}x^3 + \frac{2}{\sqrt{3}}x^4 + (p+2q)x^4 + \frac{\sqrt{5}}{\sqrt{6}}(6p+8q-9)x^5 + \frac{\sqrt{6}}{3}(15pq-9p-13q+7)x^6,$

- $S_x^{1/2}JD_y^{1/2}D_x^{1/2}[M(\Upsilon;x,y)]$
$= S_x^{1/2}JD_y^{1/2}D_x^{1/2}[xy^2 + xy^3 + (p+2q)x^2y^2 + (6p+8q-9)x^2y^3 + (15pq-9p-13q+7)x^3y^3]$
$= S_x^{1/2}JD_y^{1/2}[xy^2 + xy^3 + \sqrt{2}(p+2q)x^2y^2 + \sqrt{2}(6p+8q-9)x^2y^3 + \sqrt{3}(15pq-9p-13q+7)x^3y^3]$
$= S_x^{1/2}J[\sqrt{2}xy^2 + \sqrt{3}xy^3 + 2(p+2q)x^2y^2 + \sqrt{6}(6p+8q-9)x^2y^3 + 3(15pq-9p-13q+7)x^3y^3]$
$= S_x^{1/2}[\sqrt{2}x^3 + \sqrt{3}x^4 + 2(p+2q)x^4 + \sqrt{6}(6p+8q-9)x^5 + 3(15pq-9p-13q+7)x^6]$
$= \frac{\sqrt{2}}{\sqrt{3}}x^3 + \frac{\sqrt{3}}{2}x^4 + (p+2q)x^4 + \frac{\sqrt{6}}{\sqrt{5}}(6p+8q-9)x^5 + \frac{3}{\sqrt{6}}(15pq-9p-13q+7)x^6.$

Therefore, the Nirmala indices of Υ is given by

(i) $N(\Upsilon) = D_x^{1/2}J[M(\Upsilon;x,y)]|_{x=1}$
$= 15\sqrt{6}pq + (2+6\sqrt{5}-9\sqrt{6})p + (4+8\sqrt{5}-13\sqrt{6})q + (2+\sqrt{3}-9\sqrt{5}+7\sqrt{6}),$

(ii) $IN_1(\Upsilon) = D_x^{1/2}JS_y^{1/2}S_x^{1/2}[M(\Upsilon;x,y)]|_{x=1}$
$= 5\sqrt{6}pq + (1+\sqrt{30}-3\sqrt{6})p + \big(2+\frac{8\sqrt{5}}{\sqrt{6}}-\frac{13\sqrt{6}}{3}\big)q + \big(\frac{\sqrt{3}}{\sqrt{2}}+\frac{2}{\sqrt{3}}-\frac{9\sqrt{5}}{\sqrt{6}}+\frac{7\sqrt{6}}{3}\big),$

(iii) $IN_2(\Upsilon) = S_x^{1/2}JD_y^{1/2}D_x^{1/2}[M(\Upsilon;x,y)]|_{x=1}$
$= \frac{15\sqrt{3}}{\sqrt{2}}pq + \big(1+\frac{6\sqrt{6}}{\sqrt{5}}-\frac{9\sqrt{3}}{\sqrt{2}}\big)p + \big(2+\frac{8\sqrt{6}}{\sqrt{5}}-\frac{13\sqrt{3}}{\sqrt{2}}\big)q + \big(\frac{\sqrt{2}}{\sqrt{3}}+\frac{\sqrt{3}}{2}-\frac{9\sqrt{6}}{\sqrt{5}}+\frac{7\sqrt{3}}{\sqrt{2}}\big).$

■

2.3 Entropy measures of Si_2C_3-*I[p,q]*

Next, we calculate the various graph entropy measures of the silicon carbide network Si_2C_3-$I[p,q]$. First, we evaluate the expression for degree-based graph entropy. Later, the mathematical form of the Nirmala indices-based entropy measures is calculated by employing the previously calculated expressions of the Nirmala indices.

- **Degree-based entropy of Si_2C_3-$I[p,q]$**

Let us take under consideration, the molecular graph of Si_2C_3-$I[p,q]$ as depicted in Figure 1 which has $n = 10pq$ vertices and $m = 15pq - 2p - 3q$ edges. Now, we utilize Table 2 in Equation (5) and obtain the mathematical form of the degree-based graph entropy of Si_2C_3-$I[p,q]$

as follows:

$$ENT_{\omega}(\Upsilon) = \log(2m) - \frac{1}{2m} \sum_{s \in V(\Upsilon)} d_{\Upsilon}(s) \log(d_{\Upsilon}(s)),$$

$$\begin{aligned} ENT_{\omega}(\Upsilon) &= \log(2(15pq - 2p - 3q)) - \frac{1}{2(15pq - 2p - 3q)} \Big[\sum_{s \in V_1(\Upsilon)} d_{\Upsilon}(s) \log(d_{\Upsilon}(s)) \\ &+ \sum_{s \in V_2(\Upsilon)} d_{\Upsilon}(s) \log(d_{\Upsilon}(s)) + \sum_{s \in V_3(\Upsilon)} d_{\Upsilon}(s) \log(d_{\Upsilon}(s)) \Big] \\ &= \log(2(15pq - 2p - 3q)) - \frac{1}{2(15pq - 2p - 3q)} \Big[2 \times 1 \times \log(1) \\ &+ 2 \times (4p + 6q - 4) \times \log(2) + 3 \times (10pq - 4p - 6q + 2) \times \log(3) \Big] \\ &= \log(2(15pq - 2p - 3q)) - \frac{(4p + 6q - 4) \times \log(2)}{(15pq - 2p - 3q)} \\ &- \frac{(30pq - 12p - 18q + 6) \times \log(3)}{2(15pq - 2p - 3q)}. \end{aligned}$$

- **Nirmala entropy of Si_2C_3-$I[p, q]$**

We know from Theorem 2.2 that the expression of the Nirmala index is given as:

$$N(\Upsilon) = 15\sqrt{6}pq + (2 + 6\sqrt{5} - 9\sqrt{6})p + (4 + 8\sqrt{5} - 13\sqrt{6})q + (2 + \sqrt{3} - 9\sqrt{5} + 7\sqrt{6}).$$

Now employing Table 3 in Equation (8), we obtain the Nirmala entropy in the following way:

$$\begin{aligned} ENT_N(\Upsilon) &= \log(N(\Upsilon)) - \frac{1}{N(\Upsilon)} \sum_{st \in E(\Upsilon)} \sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)} \times \log\left(\sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)}\right) \\ &= \log(N(\Upsilon)) - \frac{1}{N(\Upsilon)} \left[\sum_{i=1}^{5} \sum_{st \in E_i(\Upsilon)} \sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)} \times \log\left(\sqrt{d_{\Upsilon}(s) + d_{\Upsilon}(t)}\right) \right] \\ &= \log(N(\Upsilon)) - \frac{1}{N(\Upsilon)} \Big[1 \times \sqrt{1+2} \times \log\left(\sqrt{1+2}\right) + 1 \times \sqrt{1+3} \times \log\left(\sqrt{1+3}\right) \\ &+ (p + 2q) \times \sqrt{2+2} \times \log\left(\sqrt{2+2}\right) + (6p + 8q - 9) \times \sqrt{2+3} \times \log\left(\sqrt{2+3}\right) \\ &+ (15pq - 9p - 13q - 7) \times \sqrt{3+3} \times \log\left(\sqrt{3+3}\right) \Big] \\ &= \log(N(\Upsilon)) - \frac{1}{N(\Upsilon)} \Big[\sqrt{3} \times \log\left(\sqrt{3}\right) + 2 \times \log(2) + 2 \times (p + 2q) \times \log(2) \\ &+ \sqrt{5} \times (6p + 8q - 9) \times \log\left(\sqrt{5}\right) + \sqrt{6} \times (15pq - 9p - 13q - 7) \times \log\left(\sqrt{6}\right) \Big]. \end{aligned}$$

Further, by substituting the value of $N(\Upsilon)$ in the above expression, we get the desired form of the Nirmala entropy of Si_2C_3-$I[p, q]$.

- **First inverse Nirmala entropy of Si_2C_3-$I[p, q]$**

The mathematical form of the first inverse Nirmala index is specified in Theorem 2.2 as

$$
\begin{aligned}
IN_1(\Upsilon) &= 5\sqrt{6}pq + (1+\sqrt{30}-3\sqrt{6})p + \left(2+\frac{8\sqrt{5}}{\sqrt{6}}-\frac{13\sqrt{6}}{3}\right)q \\
&+ \left(\frac{\sqrt{3}}{\sqrt{2}}+\frac{2}{\sqrt{3}}-\frac{9\sqrt{5}}{\sqrt{6}}+\frac{7\sqrt{6}}{3}\right).
\end{aligned}
$$

Now using Table 3 in Equation (9), we get the first inverse Nirmala entropy as follows:

$$
\begin{aligned}
ENT_{IN_1}(\Upsilon) &= \log(IN_1(\Upsilon)) - \frac{1}{IN_1(\Upsilon)} \sum_{st\in E(\Upsilon)} \sqrt{\frac{1}{d_\Upsilon(s)}+\frac{1}{d_\Upsilon(t)}} \times \log\left(\sqrt{\frac{1}{d_\Upsilon(s)}+\frac{1}{d_\Upsilon(t)}}\right) \\
&= \log(IN_1(\Upsilon)) - \frac{1}{IN_1(\Upsilon)}\left[\sum_{i=1}^{5}\sum_{st\in E_i(\Upsilon)} \sqrt{\frac{1}{d_\Upsilon(s)}+\frac{1}{d_\Upsilon(t)}} \times \log\left(\sqrt{\frac{1}{d_\Upsilon(s)}+\frac{1}{d_\Upsilon(t)}}\right)\right] \\
&= \log(IN_1(\Upsilon)) - \frac{1}{IN_1(\Upsilon)}\left[1\times\sqrt{\frac{1}{1}+\frac{1}{2}}\times\log\left(\sqrt{\frac{1}{1}+\frac{1}{2}}\right) + 1\times\sqrt{\frac{1}{1}+\frac{1}{3}}\right. \\
&\times \log\left(\sqrt{\frac{1}{1}+\frac{1}{3}}\right) + (p+2q)\times\sqrt{\frac{1}{2}+\frac{1}{2}}\times\log\left(\sqrt{\frac{1}{2}+\frac{1}{2}}\right) + (6p+8q-9) \\
&\left.\times\sqrt{\frac{1}{2}+\frac{1}{3}}\times\log\left(\sqrt{\frac{1}{2}+\frac{1}{3}}\right) + (15pq-9p-13q-7)\times\sqrt{\frac{1}{3}+\frac{1}{3}}\times\log\left(\sqrt{\frac{1}{3}+\frac{1}{3}}\right)\right] \\
&= \log(IN_1(\Upsilon)) - \frac{1}{IN_1(\Upsilon)}\left[\sqrt{\frac{3}{2}}\times\log\left(\sqrt{\frac{3}{2}}\right) + \sqrt{\frac{4}{3}}\times\log\left(\sqrt{\frac{4}{3}}\right) + (6p+8q-9)\right. \\
&\left.\times\sqrt{\frac{5}{6}}\times\log\left(\sqrt{\frac{5}{6}}\right) + (15pq-9p-13q-7)\times\sqrt{\frac{2}{3}}\times\log\left(\sqrt{\frac{2}{3}}\right)\right].
\end{aligned}
$$

Next, on putting the value of $IN_1(\Upsilon)$ in the above mathematical form, we obtain the final expression of the first inverse Nirmala entropy of Si_2C_3-$I[p,q]$.

- **Second inverse Nirmala entropy of Si_2C_3-$I[p,q]$**

The value of the second inverse Nirmala index of Si_2C_3-$I[p,q]$ calculated in Theorem 2.2 is stated below as:

$$
\begin{aligned}
IN_2(\Upsilon) &= \frac{15\sqrt{3}}{\sqrt{2}}pq + \left(1+\frac{6\sqrt{6}}{\sqrt{5}}-\frac{9\sqrt{3}}{\sqrt{2}}\right)p + \left(2+\frac{8\sqrt{6}}{\sqrt{5}}-\frac{13\sqrt{3}}{\sqrt{2}}\right)q \\
&+ \left(\frac{\sqrt{2}}{\sqrt{3}}+\frac{\sqrt{3}}{2}-\frac{9\sqrt{6}}{\sqrt{5}}+\frac{7\sqrt{3}}{\sqrt{2}}\right).
\end{aligned}
$$

Next utilizing Table 3 in Equation (10), we have the second inverse Nirmala entropy as follows:

$$\begin{aligned}
ENT_{IN_2}(\Upsilon) &= \log(IN_2(\Upsilon)) - \frac{1}{IN_2(\Upsilon)} \sum_{st\in E(\Upsilon)} \frac{\sqrt{d_\Upsilon(s)d_\Upsilon(t)}}{\sqrt{d_\Upsilon(s)+d_\Upsilon(t)}} \times \log\left(\frac{\sqrt{d_\Upsilon(s)d_\Upsilon(t)}}{\sqrt{d_\Upsilon(s)+d_\Upsilon(t)}}\right) \\
&= \log(IN_2(\Upsilon)) - \frac{1}{IN_2(\Upsilon)} \left[\sum_{i=1}^{5} \sum_{st\in E_i(\Upsilon)} \frac{\sqrt{d_\Upsilon(s)d_\Upsilon(t)}}{\sqrt{d_\Upsilon(s)+d_\Upsilon(t)}} \times \log\left(\frac{\sqrt{d_\Upsilon(s)d_\Upsilon(t)}}{\sqrt{d_\Upsilon(s)+d_\Upsilon(t)}}\right)\right] \\
&= \log(IN_2(\Upsilon)) - \frac{1}{IN_2(\Upsilon)} \left[1 \times \frac{\sqrt{1\times 2}}{\sqrt{1+2}} \times \log\left(\frac{\sqrt{1\times 2}}{\sqrt{1+2}}\right) + 1 \times \frac{\sqrt{1\times 3}}{\sqrt{1+3}}\right. \\
&\times \log\left(\frac{\sqrt{1\times 3}}{\sqrt{1+3}}\right) + (p+2q) \times \frac{\sqrt{2\times 2}}{\sqrt{2+2}} \times \log\left(\frac{\sqrt{2\times 2}}{\sqrt{2+2}}\right) + (6p+8q-9) \\
&\left.\times \frac{\sqrt{2\times 3}}{\sqrt{2+3}} \times \log\left(\frac{\sqrt{2\times 3}}{\sqrt{2+3}}\right) + (15pq-9p-13q-7) \times \frac{\sqrt{3\times 3}}{\sqrt{3+3}} \times \log\left(\frac{\sqrt{3\times 3}}{\sqrt{3+3}}\right)\right] \\
&= \log(IN_2(\Upsilon)) - \frac{1}{IN_2(\Upsilon)} \left[\frac{\sqrt{2}}{\sqrt{3}} \times \log\left(\frac{\sqrt{2}}{\sqrt{3}}\right) + \frac{\sqrt{3}}{2} \times \log\left(\frac{\sqrt{3}}{2}\right) + (6p+8q-9)\right. \\
&\left.\times \frac{\sqrt{6}}{\sqrt{5}} \times \log\left(\frac{\sqrt{6}}{\sqrt{5}}\right) + (15pq-9p-13q-7) \times \frac{\sqrt{3}}{\sqrt{2}} \times \log\left(\frac{\sqrt{3}}{\sqrt{2}}\right)\right].
\end{aligned}$$

Now, make use of $IN_2(\Upsilon)$ in the above expression, and we get the desired expression of the second inverse Nirmala entropy of Si_2C_3-$I[p,q]$.

3 Comparison through numerical and graphical demonstrations

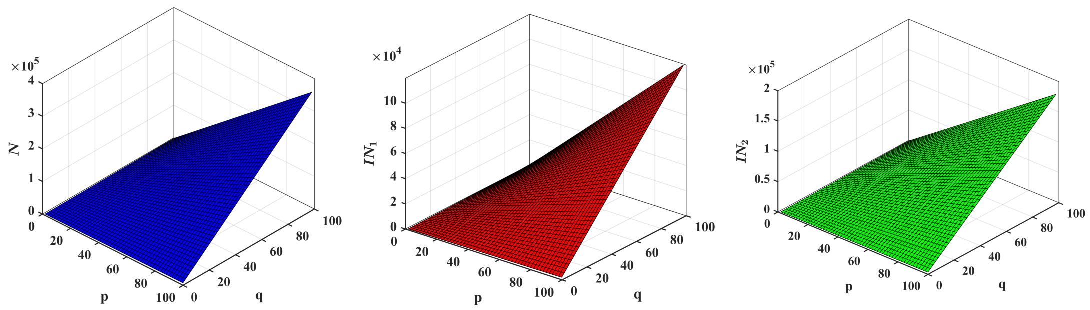
Graph entropy measures have several applications in numerous scientific areas including computer science, information theory, chemistry, biological drugs, and pharmaceuticals. Therefore the numerical computation and graphical demonstration of these molecular descriptors are subsidiaries of the scientists working in these areas. In this section, we present the comparison of the Nirmala indices and corresponding entropy measures through numerical computation, surface depiction, and $3D$ line plots. Numerical computation of the Nirmala indices and their allied entropy measures of Si_2C_3-$I[p,q]$ are tabulated in Table 4 for $1 \leq p,q \leq 50$ with condition $p=q$. Further, the surface plots of the molecular descriptors under investigation are presented in Figures 2 and 3 for $1 \leq p,q \leq 100$. Also, the comparison between the Nirmala indices and concerned entropy measures is exhibited in Figure 4 through the surface and $3D$ line plots for $1 \leq p,q \leq 100$. Table 4 and Figures 2 to 4 induce us to make the following remarks.

Remark 1. From Table 4 and Figures 2 and 3, we may observe that the Nirmala indices and associated entropy measures of silicon carbide network Si_2C_3-$I[p,q]$ increase as the values of p and q increase.

Remark 2. For silicon carbide network $\Upsilon = Si_2C_3$-$I[p,q]$, from Table 4 and Figure 4, we have the following inequality relationships $IN_1(\Upsilon) < IN_2(\Upsilon) < N(\Upsilon)$ and $ENT_{IN_1}(\Upsilon) \approx ENT_{IN_2}(\Upsilon) \approx ENT_N(\Upsilon)$.

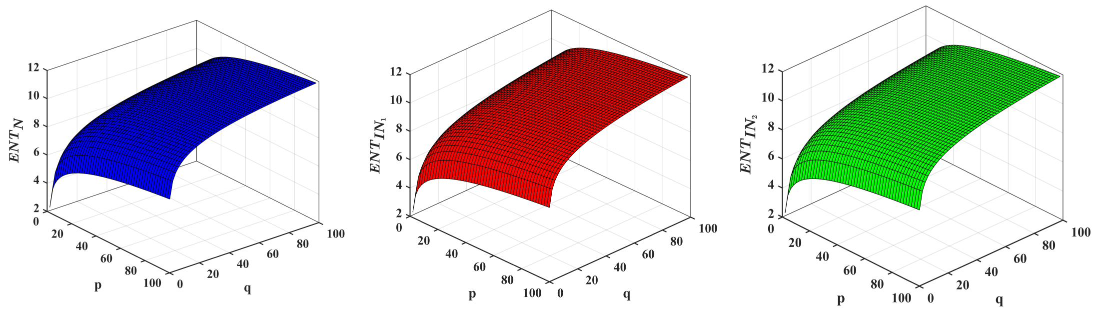
Table 4: Calculated values of the Nirmala indices and their associated entropy measures of Si_2C_3-$I[p,q]$ where $1 \leq p,q \leq 50$ with $p = q$.

$[p,q]$	N	IN_1	IN_2	ENT_N	ENT_{IN_1}	ENT_{IN_2}
[1, 1]	20.91239	9.94380	10.15975	2.29946	2.29712	2.29784
[2, 2]	114.55561	44.50341	56.66511	3.90901	3.90733	3.90801
[3, 3]	281.68351	103.55793	139.91282	4.78531	4.78413	4.78467
[4, 4]	522.29611	187.10733	259.90288	5.39194	5.39103	5.39147
[5, 5]	836.39341	295.15164	416.63528	5.85656	5.85583	5.85619
[6, 6]	1223.97539	427.69085	610.11003	6.23325	6.23264	6.23295
[7, 7]	1685.04207	584.72495	840.32712	6.55008	6.54956	6.54982
[8, 8]	2219.59344	766.25395	1107.28656	6.82349	6.82303	6.82327
[9, 9]	2827.62950	972.27784	1410.98835	7.06398	7.06356	7.06377
[10, 10]	3509.15025	1202.79664	1751.43248	7.27861	7.27824	7.27843
[11, 11]	4264.15570	1457.81033	2128.61896	7.47242	7.47209	7.47226
[12, 12]	5092.64584	1737.31892	2542.54779	7.64910	7.64879	7.64895
[13, 13]	5994.62067	2041.32240	2993.21896	7.81143	7.81114	7.81129
[14, 14]	6970.08019	2369.82079	3480.63247	7.96156	7.96129	7.96143
[15, 15]	8019.02441	2722.81407	4004.78834	8.10120	8.10095	8.10108
[16, 16]	9141.45332	3100.30225	4565.68655	8.23173	8.23149	8.23162
[17, 17]	10337.36692	3502.28532	5163.32710	8.35425	8.35403	8.35415
[18, 18]	11606.76521	3928.76329	5797.71000	8.46970	8.46949	8.46961
[19, 19]	12949.64819	4379.73616	6468.83525	8.57885	8.57866	8.57876
[20, 20]	14366.01587	4855.20393	7176.70285	8.68235	8.68216	8.68226
[21, 21]	15855.86824	5355.16659	7921.31279	8.78075	8.78057	8.78067
[22, 22]	17419.2053	5879.62416	8702.66507	8.87454	8.87437	8.87446
[23, 23]	19056.02706	6428.57662	9520.75971	8.96413	8.96396	8.96405
[24, 24]	20766.3335	7002.02398	10375.59669	9.04987	9.04972	9.04979
[25, 25]	22550.12464	7599.96623	11267.17601	9.13209	9.13194	9.13202
[26, 26]	24407.40047	8222.40339	12195.49768	9.21106	9.21092	9.21099
[27, 27]	26338.16099	8869.33544	13160.5617	9.28703	9.28689	9.28697
[28, 28]	28342.40621	9540.76238	14162.36806	9.36023	9.36009	9.36016
[29, 29]	30420.13612	10236.68423	15200.91677	9.43083	9.43070	9.43077
[30, 30]	32571.35072	10957.10097	16276.20783	9.49903	9.49891	9.49897
[31, 31]	34796.05001	11702.01261	17388.24123	9.56498	9.56486	9.56492
[32, 32]	37094.23399	12471.41915	18537.01698	9.62882	9.62871	9.62877
[33, 33]	39465.90267	13265.32058	19722.53507	9.69069	9.69058	9.69064
[34, 34]	41911.05604	14083.71692	20944.79551	9.75071	9.75059	9.75065
[35, 35]	44429.6941	14926.60815	22203.7983	9.80897	9.80886	9.80892
[36, 36]	47021.81685	15793.99427	23499.54343	9.86558	9.86548	9.86554
[37, 37]	49687.4243	16685.8753	24832.03091	9.92064	9.92054	9.92059
[38, 38]	52426.51643	17602.25122	26201.26073	9.97422	9.97412	9.97418
[39, 39]	55239.09327	18543.12204	27607.2329	10.0264	10.02631	10.02636
[40, 40]	58125.15479	19508.48775	29049.94742	10.07726	10.07717	10.07722
[41, 41]	61084.701	20498.34837	30529.40428	10.12685	10.12676	10.12681
[42, 42]	64117.73191	21512.70388	32045.60349	10.17525	10.17516	10.17521
[43, 43]	67224.24751	22551.55429	33598.54505	10.22250	10.22241	10.22246
[44, 44]	70404.2478	23614.8996	35188.22895	10.26866	10.26858	10.26862
[45, 45]	73657.73278	24702.7398	36814.6552	10.31378	10.31369	10.31374
[46, 46]	76984.70246	25815.0749	38477.82379	10.35790	10.35782	10.35786
[47, 47]	80385.15683	26951.9049	40177.73473	10.40107	10.40099	10.40104
[48, 48]	83859.09589	28113.22979	41914.38802	10.44333	10.44325	10.44329
[49, 49]	87406.51964	29299.04959	43687.78365	10.48472	10.48464	10.48468
[50, 50]	91027.42809	30509.36428	45497.92163	10.52526	10.52519	10.52523



(a) $N(\Upsilon)$ (b) $IN_1(\Upsilon)$ (c) $IN_2(\Upsilon)$

Figure 2: Graphical depiction of the Nirmala indices of $\Upsilon = Si_2C_3\text{-}I[p,q]$ for $1 \leq p,q \leq 100$.



(a) $ENT_{N(\Upsilon)}$ (b) $ENT_{IN_1(\Upsilon)}$ (c) $ENT_{IN_2(\Upsilon)}$

Figure 3: Surface plots of the Nirmala indices-based entropy measures of $\Upsilon = Si_2C_3\text{-}I[p,q]$ for $1 \leq p,q \leq 100$.

4 Curve fitting and correlation between indices and entropy measures

Curve fitting is one of the most effective and widely used data analysis methods. It is utilized to analyze the relationship between one or more independent variables and a dependent variable with the objective to develop the best-fit relationship model. Polynomial, linear, rational, and power are various methods of curve fitting. Here, we execute the curve fitting analysis to inspect the relationship between the Nirmala indices and entropy measures of $Si_2C_3\text{-}I[p,q]$ for $1 \leq p,q \leq 100$ with $p = q$. The power-2 regression model is employed to perform this data analysis.

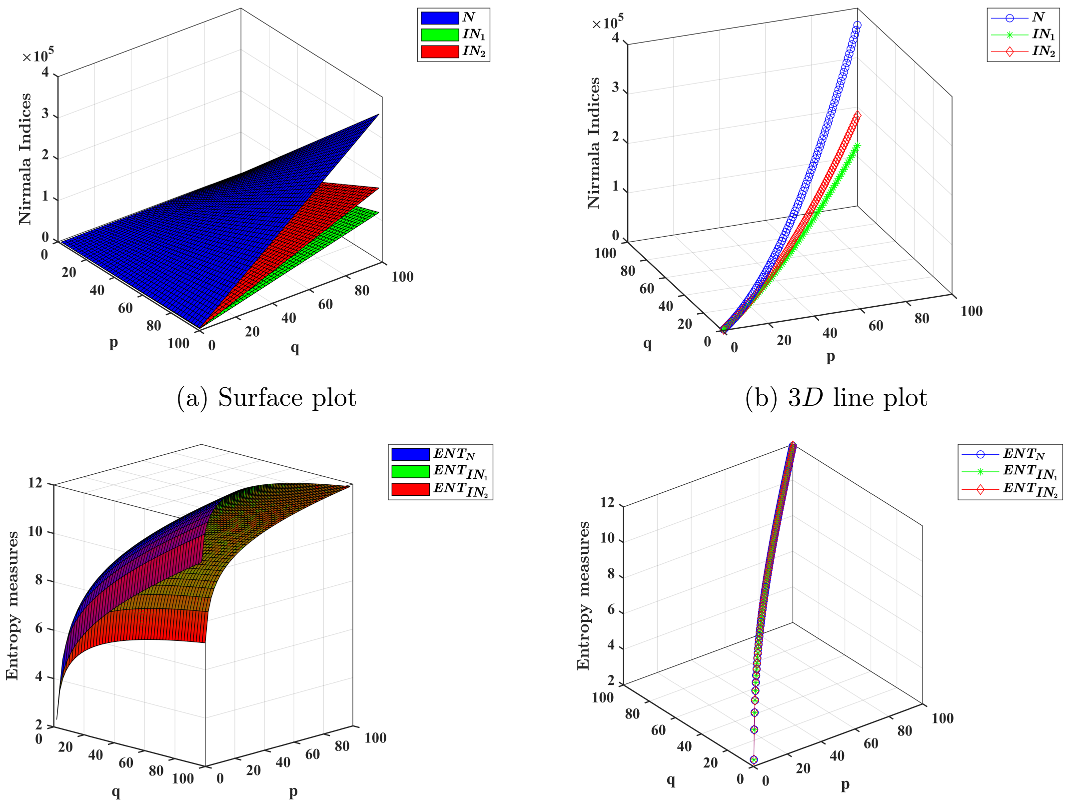
(a) General model power-2:

$$ENT_N = \alpha_1 \cdot N^{\beta_1} + \gamma_1,$$

where coefficients (with 95% confidence bounds (CB)) are $\alpha_1 = 241.8$ with CB $(217.3, 266.4)$, $\beta_1 = 0.003959$ with CB $(0.003571, 0.004347)$ and $\gamma_1 = -242.5$ with CB $(-267.1, -217.9)$.

(b) General model power-2:

$$ENT_{IN_1} = \alpha_2 \cdot {IN_1}^{\beta_2} + \gamma_2,$$



(a) Surface plot (b) $3D$ line plot

(c) Surface plot (d) $3D$ line plot

Figure 4: Comparison of the Nirmala indices and their associated entropy measures of Si_2C_3-$I[p,q]$ through surface plot and $3D$ line plot for $1 \leq p, q \leq 100$.

where coefficients (with 95% confidence bounds (CB)) are $\alpha_2 = -194.6$ with CB $(-212.1, -177)$, $\beta_2 = -0.005426$ with CB $(-0.005939, -0.004913)$ and $\gamma_2 = 194.5$ with CB $(176.9, 212.1)$.

(c) General model power-2:

$$ENT_{IN_2} = \alpha_3 \cdot {IN_2}^{\beta_3} + \gamma_3,$$

where coefficients (with 95% confidence bounds (CB)) are $\alpha_3 = 205.8$ with CB $(184.5, 227)$, $\beta_3 = 0.004634$ with CB $(0.004173, 0.005095)$ and $\gamma_3 = -205.7$ with CB $(-227, -184.4)$.

The statistical measures that are involved in the analysis, are the squared of correlation coefficient (R^2), the sum of square error (SSE), and root mean squared error ($RMSE$). The model performs efficiently if the value of $RMSE$ is low (closer to 0) and simultaneously, the higher value of R^2 (closer to 1) signifies that the regression line better fits the data. In this context, our primary focus is to obtain a lower $RMSE$ value. The curve fitting tool available in MATLAB is used to establish the regression models. The obtained statistics of fits are cataloged in Table 5 and performed models are shown in Figure 5.

Correlation analysis is a very efficient and successful data analysis tool in statistics that is used to establish the correlation between two or more data sets. Here, the correlation analysis

Table 5: Statistics of curve fitting of the Nirmala indices vs. Nirmala entropy measures of Si_2C_3-$I[p,q]$.

Topological indices	Data	Fit-type	R^2	SSE	$RMSE$
N	N vs. ENT_N	Power-2	1	0.002599	0.005176
IN_1	IN_1 vs. ENT_{IN_1}	Power-2	1	0.004260	0.006627
IN_2	IN_2 vs. ENT_{IN_2}	Power-2	1	0.003687	0.006165

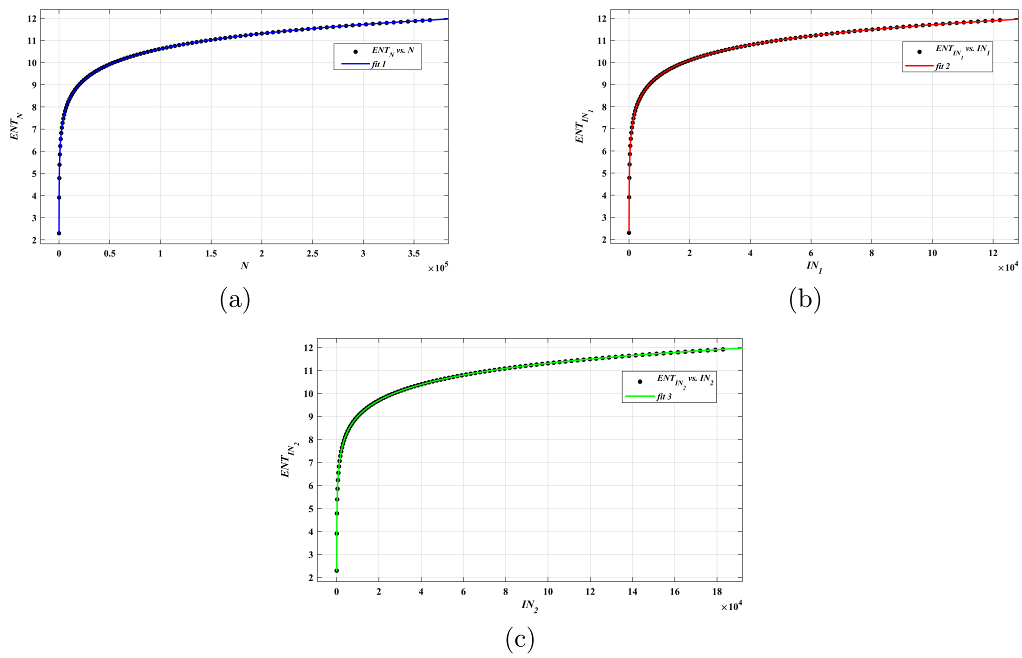


Figure 5: Curve fitting plots for the Nirmala indices vs. associated entropy measures of Si_2C_3-$I[p,q]$ for $1 \leq p,q \leq 100$ with $p = q$.

is performed to test the correlation among the Nirmala indices and allied entropy measures of Si_2C_3-$I[p,q]$ for $1 \leq p,q \leq 100$ with $p = q$. The tested value of the measure of relationship (correlation coefficient (R)) is listed in Table 6. Since the calculated values of the Nirmala indices

Table 6: Correlation among the Nirmala indices and associated entropy measures of the Si_2C_3-$I[p,q]$ network for $1 \leq p,q \leq 100$ with $p = q$.

	N	IN_1	IN_2	ENT_N	ENT_{IN_1}	ENT_{IN_2}
N	1	**0.9999**	**0.9999**	0.7718	0.7718	0.7718
IN_1	**0.9999**	1	**0.9999**	0.7722	0.7721	0.7722
IN_2	**0.9999**	**0.9999**	1	0.7718	0.7717	0.7718
ENT_N	0.7718	0.7722	0.7718	1	**0.9999**	**0.9999**
ENT_{IN_1}	0.7718	0.7721	0.7717	**0.9999**	1	**0.9999**
ENT_{IN_2}	0.7718	0.7722	0.7718	**0.9999**	**0.9999**	1

reported in Table 4 are different from each other the correlation coefficient between them is

$R = 0.9999$ which implies that they are highly correlated with each other. This concludes that these indices will predict the same structural features and properties of Si_2C_3-$I[p,q]$. Also, the Nirmala indices-based entropy measures are strongly correlated with each other with the R-value 0.9999. Therefore, a similar conclusion can be made for the Nirmala indices-based entropy measures. The above discussion suggests that the researchers may proceed with one of the Nirmala indices and one of the associated entropy measures in future research for the Si_2C_3-$I[p,q]$ network.

5 Conclusion

In this current study, we introduced three novel graph entropy measures by using new information functions based on the definitions of the Nirmala indices and named them Nirmala indices-based entropy measures. Here, the mathematical expressions of the Nirmala indices of the silicon carbide network Si_2C_3-$I[p,q]$ have been evaluated with the help of its M-polynomial to calculate the Nirmala indices-based entropy measures of this compound. Further, the numerical computation and surface depiction of the Nirmala indices and associated entropy measures have been exhibited, and we performed their comparison through the surface and $3D$ line plots. Figures 2 to 4 and Table 4 recommended that the values of the Nirmala indices and associated entropy measures of silicon carbide network Si_2C_3-$I[p,q]$ increase as the values of p and q increase and have the following relationships:

$$IN_1(\Upsilon) < IN_2(\Upsilon) < N(\Upsilon) \quad \text{and} \quad ENT_{IN_1}(\Upsilon) \approx ENT_{IN_2}(\Upsilon) \approx ENT_N(\Upsilon).$$

Additionally, the best-fit regression models between the Nirmala indices and allied entropies have been established using the curve-fitting tool in MATLAB R2019a software. Following that, the correlation analysis between the employed molecular descriptors has been performed to test their correlation with each other. The outcomes obtained in Table 6 evinced us that among six molecular descriptors, the researchers might consider one Nirmala index and one associated entropy measure in the future experimentation of this compound. The results obtained from this study would be helpful in the fields of electronic, mechanical, optical, and nanoelectronic technology to investigate the structural characteristics and topology of the silicon carbide network Si_2C_3-$I[p,q]$.

Conflicts of Interest. The authors declare that they have no conflicts of interest regarding the publication of this article.

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