

Reduced Reverse Topological Indices and Entropy Measures of Tetracyanobenzene MOFs

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Abstract: Modern material research relies heavily on metal-organic frameworks (MOFs), which are known for their highly porous and structurally tunable architectures, as well as their significance in drug delivery, gas storage, and catalysis. Topological indices (*TIs*) are numerical parameters that are graph invariant and describe the topology of a graph. In quantitative structure-property relationship (QSPR) and quantitative structure-activity relationship (QSAR) analysis, these topological indices and entropy measures (*Es*), obtained using these topological indices, help in predicting the physicochemical properties of compounds. In this study, we derive closed formulae for several reduced reverse ($\mathcal{RR}$) degree-based topological indices and their corresponding entropy measures of the Tetracyanobenzene (*TCNB*) metal-organic framework $TCNB(p, q)$. In order to prove the essential significance and validate the obtained results, we additionally perform a graphical and comparative analysis between these indices for various values of p and q .

Keywords: tetracyanobenzene metal-organic framework; topological indices; graph entropies; reduced reverse degree-based topological indices; reduced reverse degree-based entropies.

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1. Introduction

Metal-organic frameworks, or MOFs, form a novel class of hybrid crystal materials that are porous in nature and composed of metal ions and organic linkers. MOFs have garnered interest from various researchers due to their unique properties and diverse applications [1-3]. Due to their strong biodegradability and biocompatibility, MOFs are also considered viable options for constructing biosensors.

MOFs have various applications, including gas storage, adsorption, and separation, due to their porous nature and large surface area. Their clearly defined structure provides specific chemical reaction conditions, which can enhance the selectivity and effectiveness of catalyst creation [4]. They are also studied for their application in medication delivery. They can

encapsulate pharmaceuticals due to their porous nature, which enables targeted distribution and controlled drug release [5, 6]. Additionally, MOFs have a wide range of uses in detection and sensing. Their ability to modify their systems in response to specific compounds makes them useful for identifying contaminants, pollution, and even disease biomarkers. MOFs are being researched for electrochemical power applications in supercapacitors and batteries. Their design may enhance the capacity and efficiency of the power storage devices [7].

Tetracyanobenzene, or *TCNB*, is a highly conjugated, electron-deficient aromatic compound widely recognized for its multifunctional properties and applications in advanced materials. MOFs incorporating *TCNB* are synthesized by reacting *TCNB* with a metal salt in a solvent, where the metal ions form an interconnected network by coordinating with the cyano groups of the *TCNB* molecules. Such MOFs are characterized by electrical conductivity, high porosity, and thermal stability, thereby contributing to a wide range of applications. Additionally, in material science, *TCNB* plays a key role as a linker molecule in the construction of MOFs. Due to its strong electron-accepting ability and multiple coordination sites, *TCNB* is capable of linking metal centers to form extended crystalline frameworks. These frameworks exhibit potential for applications in gas storage, molecular recognition, catalysis, and optical materials. Further, *TCNB* is well-known for forming charge-transfer complexes with electron donors, enabling the design of conductive materials, organic semiconductors, and nonlinear optical systems. Moreover, in chemical graph theory, *TCNB* provides ideal case studies due to their symmetry and substituent patterns. For related work on MOFs and their applications, we cite [8-18].

A graph $\mathcal{G} = (V, E)$ is a discrete structure, with the vertex set V and the edge set E , with every element $uv \in E$ representing an edge between the vertices $u, v \in V$. The degree d_u of a vertex $u \in V$ is defined as the number of vertices adjacent to it in $\mathcal{G}$. As defined in [19], the reverse vertex degree $\mathcal{R}(u)$ of a vertex $u \in V$ is defined as $\mathcal{R}(u) = \Delta(\mathcal{G}) - d_u + 1$, where $\Delta(\mathcal{G})$ is the maximum degree of any vertex in $\mathcal{G}$. Further, the reduced reverse vertex degree of u [20], denoted $\mathcal{RR}(u)$, is defined as:

$$\mathcal{RR}(u) = \Delta(\mathcal{G}) - d_u + 2 \quad (1)$$

The topological properties of a complex chemical or molecular structure can be analyzed effectively by representing the structure as a graph, where atoms are represented by vertices and the connections between them are represented by edges. Topological indices (*TIs*), or molecular descriptors, are graph invariants, used to assess the various physico-chemical properties of the respective chemical compounds by means of the structural properties of the underlying graphs. These indices depend on various aspects of the graph, including vertex degree, distance, and graph spectrum. Some of the commonly studied *TIs* in literature are the Wiener index $W(\mathcal{G})$, Hosoya index $Z(\mathcal{G})$, Zagreb indices $M_1(\mathcal{G})$, $M_2(\mathcal{G})$, Randić index $R(\mathcal{G})$, Atom-bond connectivity index $ABC(\mathcal{G})$, Sum connectivity index $SCI(\mathcal{G})$, Symmetric division degree index $SDDI(\mathcal{G})$, Harmonic index $HM(\mathcal{G})$, Quadratic-Geometric index $QG(\mathcal{G})$, Nirmala index $N(\mathcal{G})$, Inverse Nirmala indices $IN_1(\mathcal{G})$, $IN_2(\mathcal{G})$, Sombor index $SO(\mathcal{G})$ and its variants. For recent studies on various topological indices and related work, we cite [21-42]. Topological indices are widely used in analyzing the physicochemical properties of chemical compounds through QSPR and QSAR analysis, which are based on the numerical relationship between chemical structures and their property values.

In 1948, Shannon [43] first proposed the concept of entropy, a measure of the uncertainty or unpredictability of the information contained in a system based on probability

distributions. In later studies, it was observed that chemical networks and graphs are analyzed to understand structural information using entropy. The graph entropy measures, obtained using topological indices, were found to be useful to assess the structural diversity of chemical compounds. In particular, higher structural diversity was indicated by higher entropy values. Particularly, degree-based entropy could be applied in various fields such as organic and inorganic chemistry, chemical graph theory, biology, and mathematics. For related work, we cite [44-51].

Based on a literature survey conducted in the domains of topological indices and graph entropy, this article presents results providing closed formulae for the reduced reverse vertex degree-based topological indices (*TIs*) and graph entropies (*Es*) of *TCNB* MOFs. Further, we provide a graphical and comparative analysis of the computed *TIs* and *Es* to provide significance to the obtained results.

2. Basic Definitions

Given a graph $\mathcal{G}$, with its vertex set $V(\mathcal{G})$ and edge set $E(\mathcal{G})$, a reduced reverse vertex degree-based topological index $\mathcal{RRTI}(\mathcal{G})$ [20] is generally defined as:

$$\mathcal{RRTI}(\mathcal{G}) = \sum_{uv \in E(\mathcal{G})} f(\mathcal{RR}(u), \mathcal{RR}(v)) \quad (2)$$

where $f(\mathcal{RR}(u), \mathcal{RR}(v))$ is a real-valued function, with $\mathcal{RR}(u)$ and $\mathcal{RR}(v)$ being the reduced reverse degrees of the vertices u and v in $\mathcal{G}$.

Based on the definition of the reduced reverse vertex degree of a vertex, various reduced reverse degree-based topological indices are defined by choosing a particular function $f(\mathcal{RR}(u), \mathcal{RR}(v))$ as follows:

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \mathcal{RR}(u) + \mathcal{RR}(v)$, then $TI(\mathcal{G})$ is the first reduced reverse Zagreb index $\mathcal{RRM}_1(\mathcal{G})$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \mathcal{RR}(u) \times \mathcal{RR}(v)$, then $TI(\mathcal{G})$ is the second reduced reverse Zagreb index $\mathcal{RRM}_2(\mathcal{G})$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \mathcal{RR}(u) - \mathcal{RR}(v)$, then $TI(\mathcal{G})$ is the third reduced reverse Zagreb index $\mathcal{RRM}_3(\mathcal{G})$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = (\mathcal{RR}(u) + \mathcal{RR}(v))^2$, then $TI(\mathcal{G})$ is the first reduced reverse hyper-Zagreb index $\mathcal{RRHM}_1(\mathcal{G})$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = (\mathcal{RR}(u) \times \mathcal{RR}(v))^2$, then $TI(\mathcal{G})$ is the second reduced reverse hyper-Zagreb index $\mathcal{RRHM}_2(\mathcal{G})$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \mathcal{RR}(u)^2 + \mathcal{RR}(v)^2$, then $TI(\mathcal{G})$ is the reduced reverse forgotten index $\mathcal{RRF}(\mathcal{G})$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \sqrt{\frac{\mathcal{RR}(u) + \mathcal{RR}(v) - 2}{\mathcal{RR}(u) \times \mathcal{RR}(v)}}$, then $TI(\mathcal{G})$ is the reduced reverse atom-bond connectivity(ABC) index $\mathcal{RRABC}(\mathcal{G})$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \frac{2\sqrt{\mathcal{RR}(u) \times \mathcal{RR}(v)}}{\mathcal{RR}(u) + \mathcal{RR}(v)}$, then $TI(\mathcal{G})$ is the reduced reverse geometric-arithmetic(GA) index $\mathcal{RRGA}(\mathcal{G})$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \frac{\mathcal{RR}(u) + \mathcal{RR}(v)}{\mathcal{RR}(u) \times \mathcal{RR}(v)}$, then $TI(\mathcal{G})$ is the first reduced reverse redefined Zagreb index $\mathcal{RR}[ReZ_1(\mathcal{G})]$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \frac{\mathcal{RR}(u) \times \mathcal{RR}(v)}{\mathcal{RR}(u) + \mathcal{RR}(v)}$, then $TI(G)$ is the second reduced reverse redefined Zagreb index $\mathcal{RR}[ReZ_2(G)]$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = (\mathcal{RR}(u) \times \mathcal{RR}(v))(\mathcal{RR}(u) + \mathcal{RR}(v))$, then $TI(G)$ is the third reduced reverse redefined Zagreb index $\mathcal{RR}[ReZ_3(G)]$.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \mathcal{RR}(u)^r \times \mathcal{RR}(v)^s + \mathcal{RR}(u)^s \times \mathcal{RR}(v)^r$, then $TI(G)$ is the reduced reverse generalized Zagreb index $\mathcal{RR}[M_{r,s}(G)]$.

3. Results and Discussion

The chemical structure of $TCNB(p, q)$ consists of $p \geq 1$ horizontal and $q \geq 1$ vertical expansions. For instance, the structure of $TCNB(1,1)$ is depicted in Figure 1. In general, the $TCNB(p, q)$ graphical structure consists of $25p + 25q + 33pq + 17$ vertices (atoms) and $32p + 32q + 44pq + 20$ edges (bonds). Furthermore, it comprises vertices of four different degrees, ranging from 1 to 4, and five edge partitions, as shown in Tables 1 and 2.

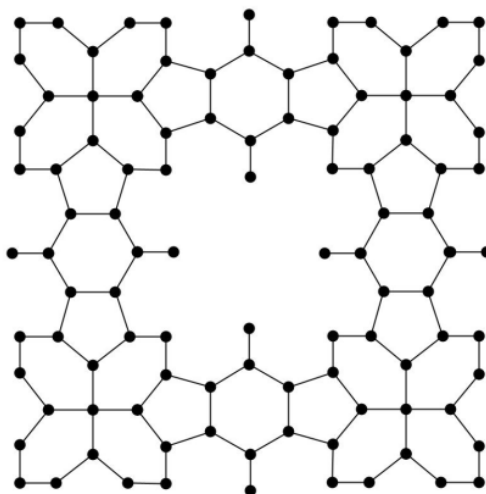


Figure 1. Molecular structure of $TCNB(1,1)$.

Table 1. Vertex partition of $TCNB(p, q)$.

d_u	$\mathcal{RR}(u)$	Frequency
1	5	$2p + 2q + 4pq$
2	4	$8p + 8q + 4pq + 12$
3	3	$14p + 14q + 24pq + 4$
4	2	$p + q + pq + 1$

Table 2. Edge partition of $TCNB(p, q)$ based on degree and reduced reverse degree of end vertices.

(d_u, d_v)	$(\mathcal{RR}(u), \mathcal{RR}(v))$	Frequency
(1, 3)	(5, 3)	$2p + 2q + 4pq$
(2, 3)	(4, 3)	$8p + 8q + 8pq + 8$
(2, 2)	(4, 4)	$4p + 4q + 8$
(3, 3)	(3, 3)	$14p + 14q + 28pq$
(3, 4)	(3, 2)	$4p + 4q + 4pq + 4$

Using these vertex and edge partitions, we propose the following result, giving the expression of any reduced reverse vertex degree-based topological index of $TCNB(p, q)$. Using the proposition, we obtain the closed forms of the expressions for various reverse vertex degree-based topological indices in the latter part of the section.

Proposition 3.1 For $G = TCNB(p, q)$, the reduced reverse vertex degree-based topological index $\mathcal{RRTI}(G)$ is given by

$$\begin{aligned}\mathcal{RRTI}(TCNB(p, q)) &= \mathcal{RRTI}(\mathcal{G}) \\ &= (2p + 2q + 4pq)f(5,3) + (8p + 8q + 8pq + 8)f(4,3) \\ &\quad + (4p + 4q + 8)f(4,4) + (14p + 14q + 28pq)f(3,3) \\ &\quad + (4p + 4q + 4pq + 4)f(3,2) \quad (3)\end{aligned}$$

Proposition 3.2 The reduced reverse Zagreb indices of $\mathcal{G} = TCNB(p, q)$ are:

$$\bullet \mathcal{RRM}_1(\mathcal{G}) = 208p + 208q + 276pq + 140 \quad (4)$$

$$\bullet \mathcal{RRM}_2(\mathcal{G}) = 340p + 340q + 432pq + 248 \quad (5)$$

$$\bullet \mathcal{RRM}_3(\mathcal{G}) = 16p + 16q + 20pq + 12. \quad (6)$$

Proof. By definition, the first reduced reverse Zagreb index of $\mathcal{G}$ is given by,

$$\begin{aligned}\mathcal{RRM}_1(\mathcal{G}) &= \sum_{uv \in E(\mathcal{G})} (\mathcal{RR}(u) + \mathcal{RR}(v)) \\ &= (2p + 2q + 4pq)(5 + 3) + (8p + 8q + 8pq + 8)(4 + 3) \\ &\quad + (4p + 4q + 8)(4 + 4) + (14p + 14q + 28pq)(3 + 3) \\ &\quad + (4p + 4q + 4pq + 4)(3 + 2) \\ &= 208p + 208q + 276pq + 140 \quad (7)\end{aligned}$$

The second reduced reverse Zagreb index of $\mathcal{G}$ is given by

$$\begin{aligned}\mathcal{RRM}_2(\mathcal{G}) &= \sum_{uv \in E(\mathcal{G})} (\mathcal{RR}(u) \times \mathcal{RR}(v)) \\ &= (2p + 2q + 4pq)(5 \times 3) + (8p + 8q + 8pq + 8)(4 \times 3) \\ &\quad + (4p + 4q + 8)(4 \times 4) + (14p + 14q + 28pq)(3 \times 3) + (4p \\ &\quad + 4q + 4pq + 4)(3 \times 2) \\ &= 340p + 340q + 432pq + 248 \quad (8)\end{aligned}$$

The third reduced reverse Zagreb index of $\mathcal{G}$ is given by,

$$\begin{aligned}\mathcal{RRM}_3(\mathcal{G}) &= \sum_{uv \in E(\mathcal{G})} (\mathcal{RR}(u) - \mathcal{RR}(v)) \\ &= (2p + 2q + 4pq)(5 - 3) + (8p + 8q + 8pq + 8)(4 - 3) + (4p + 4q + 8)(4 \\ &\quad - 4) \\ &\quad + (14p + 14q + 28pq)(3 - 3) + (4p + 4q + 4pq + 4)(3 - 2) \\ &= 16p + 16q + 20pq + 12 \quad (9)\end{aligned}$$

Proposition 3.3 The reduced reverse hyper-Zagreb indices of $\mathcal{G} = TCNB(p, q)$ are:

$$\bullet \mathcal{RRHM}_1(\mathcal{G}) = 1380p + 1380q + 1756pq + 1004 \quad (10)$$

$$\bullet \mathcal{RRHM}_2(\mathcal{G}) = 3904p + 3904q + 4464pq + 3344 \quad (11)$$

Proof. The first reduced reverse hyper-Zagreb index of $\mathcal{G}$ is given by,

$$\begin{aligned}\mathcal{RRHM}_1(\mathcal{G}) &= \sum_{uv \in E(\mathcal{G})} (\mathcal{RR}(u) + \mathcal{RR}(v))^2 \\ &= (2p + 2q + 4pq)(5 + 3)^2 + (8p + 8q + 8pq + 8)(4 + 3)^2 + (4p + 4q + 8) \\ &\quad (4 + 4)^2 + (14p + 14q + 28pq)(3 + 3)^2 + (4p + 4q + 4pq + 4)(3 + 2)^2 \\ &= 1380p + 1380q + 1756pq + 1004 \quad (12)\end{aligned}$$

The second reduced reverse hyper-Zagreb index of $\mathcal{G}$ is given by

$$\begin{aligned}\mathcal{RRHM}_2(\mathcal{G}) &= \sum_{uv \in E(\mathcal{G})} (\mathcal{G}) \Rightarrow \times \mathcal{RR}(v))^2 \\ &= (2p + 2q + 4pq)(5 \times 3)^2 + (8p + 8q + 8pq + 8)(4 \times 3)^2 + (4p + 4q + 8) \\ &\quad (4 \times 4)^2 + (14p + 14q + 28pq)(3 \times 3)^2 + (4p + 4q + 4pq + 4)(3 \times 2)^2 \\ &= 3904p + 3904q + 4464pq + 3344 \quad (13)\end{aligned}$$

Proposition 3.4 The reduced reverse forgotten index, atom-bond connectivity (ABC) index, and geometric-arithmetic (GA) index of $\mathcal{G} = TCNB(p, q)$ are:

$$\bullet \mathcal{RRF}(\mathcal{G}) = 700p + 700q + 892pq + 308 \quad (14)$$

$$\bullet \mathcal{RRABC}(\mathcal{G}) = 21.0408p + 21.0408q + 29.19pq + 12.89 \quad (15)$$

$$\bullet \mathcal{RRGA}(\mathcal{G}) = 31.7736p + 31.7736q + 43.7101pq + 19.8371 \quad (16)$$

Proof. The reduced reverse forgotten index of $\mathcal{G}$ is given by

$$\begin{aligned}\mathcal{RRF}(\mathcal{G}) &= \sum_{uv \in E(\mathcal{G})} (\mathcal{RR}(u)^2 + \mathcal{RR}(v)^2) \\ &= (2p + 2q + 4pq)(5^2 + 3^2) + (8p + 8q + 8pq + 8)(4^2 + 3^2) + (4p + 4q + 8) \\ &\quad (4^2 + 4^2) + (14p + 14q + 28pq)(3^2 + 3^2) + (4p + 4q + 4pq + 4)(3^2 + 2^2) \\ &= 700p + 700q + 892pq + 308 \quad (17)\end{aligned}$$

The reduced reverse ABC index of $\mathcal{G}$ is given by

$$\begin{aligned}\mathcal{RRABC}(\mathcal{G}) &= \sum_{uv \in E(\mathcal{G})} \left(\sqrt{\frac{\mathcal{RR}(u) + \mathcal{RR}(v) - 2}{\mathcal{RR}(u) \times \mathcal{RR}(v)}} \right) \\ &= (2p + 2q + 4pq) \left(\sqrt{\frac{5+3-2}{5 \times 3}} \right) + (8p + 8q + 8pq + 8) \left(\sqrt{\frac{4+3-2}{4 \times 3}} \right) \\ &\quad + (4p + 4q + 8) \left(\sqrt{\frac{4+4-2}{4 \times 4}} \right) + (14p + 14q + 28pq) \left(\sqrt{\frac{3+3-2}{3 \times 3}} \right) \\ &\quad + (4p + 4q + 4pq + 4) \left(\sqrt{\frac{3+2-2}{3 \times 2}} \right) \\ &= 21.0408p + 21.0408q + 29.19pq + 12.89 \quad (18)\end{aligned}$$

The reduced reverse GA index of $\mathcal{G}$ is given by

$$\begin{aligned}\mathcal{RRGA}(\mathcal{G}) &= \sum_{uv \in E(\mathcal{G})} \left(\frac{2\sqrt{\mathcal{RR}(u) \times \mathcal{RR}(v)}}{\mathcal{RR}(u) + \mathcal{RR}(v)} \right) \\ &= (2p + 2q + 4pq) \left(\frac{2\sqrt{5 \times 3}}{5 + 3} \right) + (8p + 8q + 8pq + 8) \left(\frac{2\sqrt{4 \times 3}}{4 + 3} \right) \\ &\quad + (4p + 4q + 8) \left(\frac{2\sqrt{4 \times 4}}{4 + 4} \right) + (14p + 14q + 28pq) \left(\frac{2\sqrt{3 \times 3}}{3 + 3} \right) \\ &\quad + (4p + 4q + 4pq + 4) \left(\frac{2\sqrt{3 \times 2}}{3 + 2} \right)\end{aligned}$$

$$= 31.7736p + 31.7736q + 43.7101pq + 19.8371. \quad (19)$$

Proposition 3.5 The reduced reverse redefined Zagreb indices of $\mathcal{G} = TCNB(p, q)$ are:

- $\mathcal{RR}[ReZ_1(\mathcal{G})] = 20.40p + 20.40q + 28.80pq + 12,$
- $\mathcal{RR}[ReZ_2(\mathcal{G})] = 51.26p + 51.26q + 68.01pq + 34.51,$
- $\mathcal{RR}[ReZ_3(\mathcal{G})] = 2300p + 2300q + 2784pq + 1816.$

Proof. The first reduced reverse redefined Zagreb index of $\mathcal{G}$ is given by,

$$\begin{aligned} \mathcal{RR}[ReZ_1(\mathcal{G})] &= \sum_{uv \in E(\mathcal{G})} \left(\frac{\mathcal{RR}(u) + \mathcal{RR}(v)}{\mathcal{RR}(u) \times \mathcal{RR}(v)} \right) \\ &= (2p + 2q + 4pq) \left(\frac{5 + 3}{5 \times 3} \right) + (8p + 8q + 8pq + 8) \left(\frac{4 + 3}{4 \times 3} \right) + (4p + 4q \\ &\quad + 8) \left(\frac{4 + 4}{4 \times 4} \right) + (14p + 14q + 28pq) \left(\frac{3 + 3}{3 \times 3} \right) + (4p + 4q + 4pq \\ &\quad + 4) \left(\frac{3 + 2}{3 \times 2} \right) \\ &= 20.40p + 20.40q + 28.80pq + 12. \end{aligned} \quad (20)$$

The second reduced reverse redefined Zagreb index of $\mathcal{G}$ is given by,

$$\begin{aligned} \mathcal{RR}[ReZ_2(\mathcal{G})] &= \sum_{uv \in E(\mathcal{G})} \left(\frac{\mathcal{RR}(u) \times \mathcal{RR}(v)}{\mathcal{RR}(u) + \mathcal{RR}(v)} \right) \\ &= (2p + 2q + 4pq) \left(\frac{5 \times 3}{5 + 3} \right) + (8p + 8q + 8pq + 8) \left(\frac{4 \times 3}{4 + 3} \right) + (4p + 4q \\ &\quad + 8) \left(\frac{4 \times 4}{4 + 4} \right) + (14p + 14q + 28pq) \left(\frac{3 \times 3}{3 + 3} \right) + (4p + 4q + 4pq \\ &\quad + 4) \left(\frac{3 \times 2}{3 + 2} \right) \\ &= 51.26p + 51.26q + 68.01pq + 34.51. \end{aligned} \quad (21)$$

The third reduced reverse redefined Zagreb index of $\mathcal{G}$ is given by,

$$\begin{aligned} \mathcal{RR}[ReZ_3(\mathcal{G})] &= \sum_{uv \in E(\mathcal{G})} (\mathcal{RR}(u) \times \mathcal{RR}(v))(\mathcal{RR}(u) + \mathcal{RR}(v)) \\ &= (2p + 2q + 4pq)(5 \times 3)(5 + 3) + (8p + 8q + 8pq + 8)(4 \times 3)(4 + 3) \\ &\quad + (4p + 4q + 8)(4 \times 4)(4 + 4) + (14p + 14q + 28pq)(3 \times 3)(3 + 3) \\ &\quad + (4p + 4q + 4pq + 4)(3 \times 2)(3 + 2) \\ &= 2300p + 2300q + 2784pq + 1816. \end{aligned} \quad (22)$$

Proposition 3.6 The reduced reverse generalized Zagreb index of $\mathcal{G} = TCNB(p, q)$ is

$$\begin{aligned} \mathcal{RR}[M_{r,s}(\mathcal{G})] &= (2p + 2q + 4pq)(5^r \times 3^s + 5^s \times 3^r) + (8p + 8q + 8pq + \\ &\quad 8)(4^r \times 3^s + 4^s \times 3^r) + (8p + 8q + 16)(4^{r+s}) + (28p + 28q + 56pq)(3^{r+s}) + (4p + \\ &\quad 4q + 4pq + 4)(3^r \times 2^s + 3^s \times 2^r). \end{aligned} \quad (23)$$

Proof. The reduced reverse generalized Zagreb index of $\mathcal{G}$ is given by

$$\begin{aligned} \mathcal{RR}[M_{r,s}(\mathcal{G})] &= \sum_{uv \in E(\mathcal{G})} (\mathcal{RR}(u)^r \times \mathcal{RR}(v)^s + \mathcal{RR}(u)^s \times \mathcal{RR}(v)^r) \\ &= (2p + 2q + 4pq)(5^r \times 3^s + 5^s \times 3^r) + (8p + 8q + 8pq + 8)(4^r \times 3^s + \\ &\quad 4^s \times 3^r) + (4p + 4q + 8)((4^r \times 4^s) + (4^s \times 4^r)) + (14p + 14q + \\ &\quad 28pq)((3^r \times 3^s) + (3^s \times 3^r)) + (4p + 4q + 4pq + 4)(3^r \times 2^s + 3^s \times 2^r) \end{aligned}$$

$$= (2p + 2q + 4pq)(5^r \times 3^s + 5^s \times 3^r) + (8p + 8q + 8pq + 8)(4^r \times 3^s + 4^s \times 3^r) + (8p + 8q + 16)(4^{r+s}) + (28p + 28q + 56pq)(3^{r+s}) + (4p + 4q + 4pq + 4)(3^r \times 2^s + 3^s \times 2^r). \quad (24)$$

Tables 3 and 4 provide the values of the topological indices discussed in the above propositions for specific values of p and q with $p = q = 1, 2, \dots, 20$. Further, Figure 2 gives the graphical interpretation of the indices for these values of p and q .

Table 3. Numerical behaviour of topological indices of $\mathcal{G} = TCNB(p, q)$ for some specific values of p and q with $p = q$.

(p, q)	$RRM_1(\mathcal{G})$	$RRM_2(\mathcal{G})$	$RRM_3(\mathcal{G})$	$RRHM_1(\mathcal{G})$	$RRHM_2(\mathcal{G})$	$RRF(\mathcal{G})$
(1, 1)	832	1360	64	5520	15616	2600
(2, 2)	2076	3336	156	13548	36816	6676
(3, 3)	3872	6176	288	25088	66944	12536
(4, 4)	6220	9880	460	40140	106000	20180
(5, 5)	9120	14448	672	58704	153984	29608
(6, 6)	12572	19880	924	80780	210896	40820
(7, 7)	16576	26176	1216	106368	276736	53816
(8, 8)	21132	33336	1548	135468	351504	68596
(9, 9)	26240	41360	1920	168080	435200	85160
(10, 10)	31900	50248	2332	204204	527824	103508
(11, 11)	38112	60000	2784	243840	629376	123640
(12, 12)	44876	70616	3276	286988	739856	145556
(13, 13)	52192	82096	3808	333648	859264	169256
(14, 14)	60060	94440	4380	383820	987600	194740
(15, 15)	68480	107648	4992	437504	1124864	222008
(16, 16)	77452	121720	5644	494700	1271056	251060
(17, 17)	86976	136656	6336	555408	1426176	281896
(18, 18)	97052	152456	7068	619628	1590224	314516
(19, 19)	107680	169120	7840	687360	1763200	348920
(20, 20)	118860	186648	8652	758604	1945104	385108

Table 4. Numerical behaviour of topological indices of $\mathcal{G} = TCNB(p, q)$ for some specific values of p and q with $p = q$.

(p, q)	$RRABC(\mathcal{G})$	$RRGA(\mathcal{G})$	$RR(ReZ_1(\mathcal{G}))$	$RR(ReZ_2(\mathcal{G}))$	$RR(ReZ_3(\mathcal{G}))$
(1, 1)	84.1616	127.0945	81.6	205.04	9200
(2, 2)	213.8132	321.7721	208.8	511.59	22152
(3, 3)	401.8448	603.8699	393.6	954.16	40672
(4, 4)	648.2564	973.3879	636	1532.75	64760
(5, 5)	953.0480	1430.3262	936	2247.36	94416
(6, 6)	1316.2196	1974.6847	1293.6	3097.99	129640
(7, 7)	1737.7712	2606.4634	1708.8	4084.64	170432
(8, 8)	2217.7028	3325.6623	2181.6	5207.31	216792
(9, 9)	2756.0144	4132.2815	2712	6466	268720
(10, 10)	3352.7060	5026.3209	3300	7860.71	326216
(11, 11)	4007.7776	6007.7805	3945.6	9391.44	389280
(12, 12)	4721.2292	7076.6604	4648.8	11058.19	457912
(13, 13)	5493.0608	8232.9605	5409.6	12860.96	532112
(14, 14)	6323.2724	9476.6808	6228	14799.75	611880
(15, 15)	7211.8640	10807.8213	7104	16874.56	697216
(16, 16)	8158.8356	12226.3821	8037.6	19085.39	788120
(17, 17)	9164.1872	13732.3631	9028.8	21432.24	884592
(18, 18)	10227.9188	15325.7643	10077.6	23915.11	986632
(19, 19)	11350.0304	17006.5857	11184	26534	1094240
(20, 20)	12530.5220	18774.8274	12348	29288.91	1207416

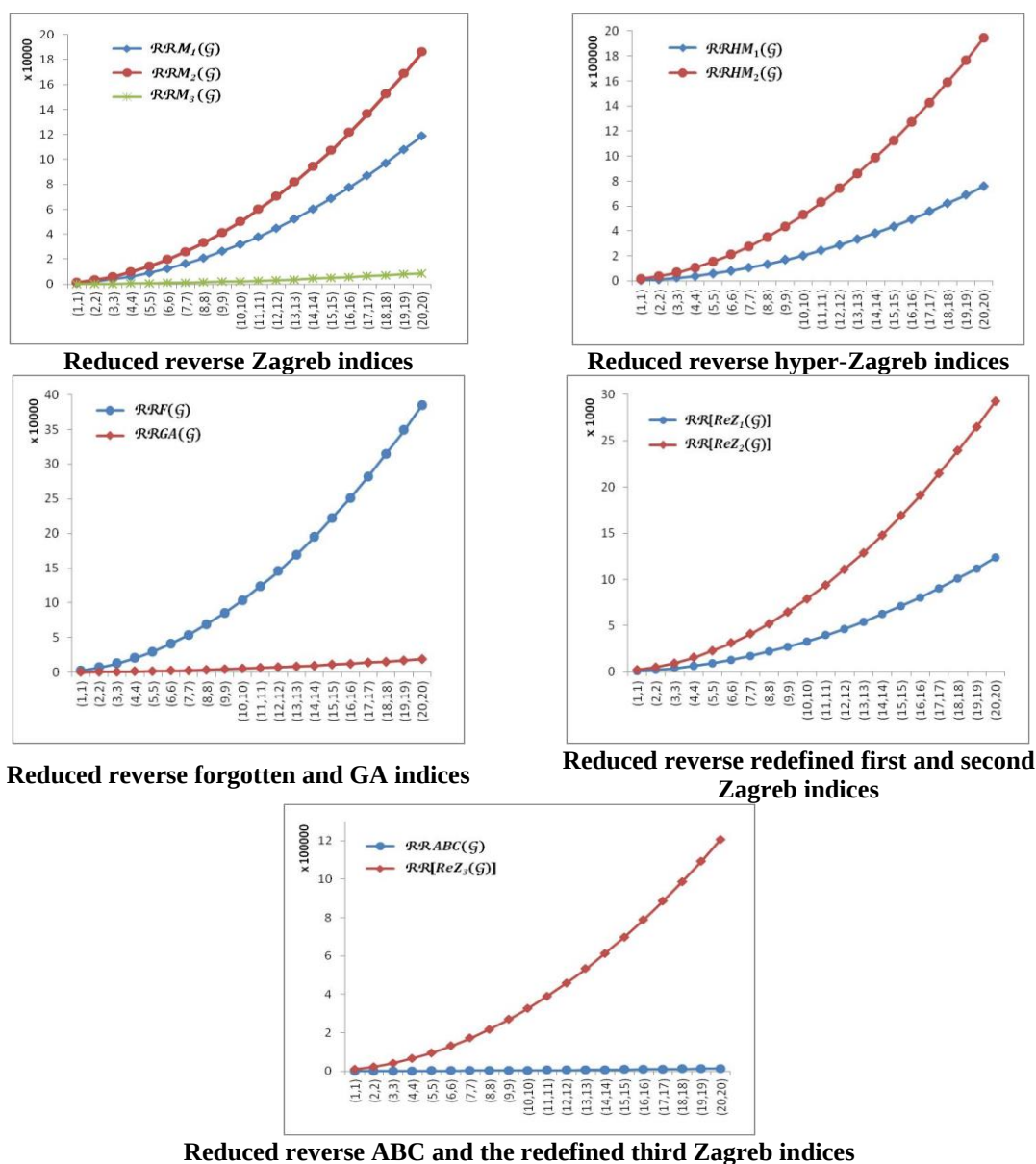


Figure 2. Graphical representation of reduced reverse degree-based topological indices of $G = TCNB(p, q)$ for some specific values of p and q with $p = q$.

4. Graph Entropy

Definition 4.1 [52] Let $G = (V, E)$ be a connected graph of order n and ϕ be an arbitrary function defined on the vertex set $V = \{v_1, v_2, \dots, v_n\}$ of G . Then the entropy of G is defined as

$$I_\phi(G) = - \sum_{i=1}^n \frac{\phi(v_i)}{\sum_{i=1}^n \phi(v_i)} \log \left(\frac{\phi(v_i)}{\sum_{i=1}^n \phi(v_i)} \right).$$

As defined in [53], the entropy of the edge-weighted graph $G = (V, E)$, with the edge weight of the edge $v_i v_j$ being $\omega(v_i v_j)$, is given by

$$\begin{aligned} \mathbb{E}(G) &= - \sum_{v_i v_j \in E} \frac{\omega(v_i v_j)}{\sum_{v_i v_j \in E} \omega(v_i v_j)} \log \left(\frac{\omega(v_i v_j)}{\sum_{v_i v_j \in E} \omega(v_i v_j)} \right) \\ &= - \frac{1}{\sum_{v_i v_j \in E} \omega(v_i v_j)} \sum_{v_i v_j \in E} \left(\omega(v_i v_j) \left[\log(\omega(v_i v_j)) - \log \left(\sum_{v_i v_j \in E} \omega(v_i v_j) \right) \right] \right) \end{aligned}$$

so that

$$\mathbb{E}(\mathcal{G}) = \log \left(\sum_{v_i v_j \in E} \omega(v_i v_j) \right) - \frac{1}{\sum_{v_i v_j \in E} \omega(v_i v_j)} \sum_{v_i v_j \in E} \left(\omega(v_i v_j) \log(\omega(v_i v_j)) \right).$$

Replacing $\sum_{v_i v_j \in E} \omega(v_i v_j)$ with $TI(\mathcal{G})$, we get the required degree-based entropy of $\mathcal{G}$ as

$$\mathbb{E}(\mathcal{G}) = \log(TI(\mathcal{G})) - \frac{1}{TI(\mathcal{G})} \sum_{v_i v_j \in E} \left(\omega(v_i v_j) \log(\omega(v_i v_j)) \right). \quad (25)$$

Reduced reverse degree-based entropy of tetracyanobenzene MOFs.

For $\mathcal{G} = TCNB(p, q)$, the reduced reverse vertex degree-based entropy $\mathbb{E}_{\mathcal{RRTI}(\mathcal{G})}$ is given by

$$\mathbb{E}_{\mathcal{RRTI}(\mathcal{G})} = \log(\mathcal{RRTI}(\mathcal{G})) - \frac{1}{\mathcal{RRTI}(\mathcal{G})} \sum_{uv \in E(\mathcal{G})} [f(\mathcal{RR}(u), \mathcal{RR}(v)) \times \log(f(\mathcal{RR}(u), \mathcal{RR}(v)))] \quad (26)$$

4.1. First reduced reverse Zagreb entropy.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \mathcal{RR}(u) + \mathcal{RR}(v)$ and $\mathcal{RRM}_1(\mathcal{G}) = 208p + 208q + 276pq + 140$, then the first reduced reverse Zagreb entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{RRM}_1(\mathcal{G})} &= \log(\mathcal{RRM}_1(\mathcal{G})) \\ &\quad - \frac{1}{\mathcal{RRM}_1(\mathcal{G})} \sum_{uv \in E(\mathcal{G})} [(\mathcal{RR}(u) + \mathcal{RR}(v)) \times \log(\mathcal{RR}(u) + \mathcal{RR}(v))] \\ &= \log(\mathcal{RRM}_1(\mathcal{G})) - \frac{1}{\mathcal{RRM}_1(\mathcal{G})} [(2p + 2q + 4pq) \times 8 \times \log 8 + (8p + 8q + 8pq + 8) \times 7 \times \log 7 \\ &\quad + (4p + 4q + 8) \times 8 \times \log 8 + (14p + 14q + 28pq) \times 6 \times \log 6 + (4p + 4q + 4pq + 4) \times 5 \times \log 5]. \end{aligned} \quad (27)$$

4.2. Second reduced reverse Zagreb entropy.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \mathcal{RR}(u) \times \mathcal{RR}(v)$ and $\mathcal{RRM}_2(\mathcal{G}) = 340p + 340q + 432pq + 248$, then the second reduced reverse Zagreb entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{RRM}_2(\mathcal{G})} &= \log(\mathcal{RRM}_2(\mathcal{G})) \\ &\quad - \frac{1}{\mathcal{RRM}_2(\mathcal{G})} \sum_{uv \in E(\mathcal{G})} [\mathcal{RR}(u) \times \mathcal{RR}(v) \times \log(\mathcal{RR}(u) \times \mathcal{RR}(v))] \\ &= \log(\mathcal{RRM}_2(\mathcal{G})) - \frac{1}{\mathcal{RRM}_2(\mathcal{G})} [(2p + 2q + 4pq) \times 15 \times \log 15 + (8p + 8q + 8pq + 8) \times 12 \times \log 12 \\ &\quad + (4p + 4q + 8) \times 16 \times \log 16 + (14p + 14q + 28pq) \times 9 \times \log 9 + (4p + 4q + 4pq + 4) \times 6 \times \log 6]. \end{aligned} \quad (28)$$

4.3. First reduced reverse hyper Zagreb entropy.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = (\mathcal{RR}(u) + \mathcal{RR}(v))^2$ and $\mathcal{RRHM}_1(\mathcal{G}) = 1380p + 1380q + 1756pq + 1004$, then the first reduced reverse hyper Zagreb entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{RRHM}_1(\mathcal{G})} &= \log(\mathcal{RRHM}_1(\mathcal{G})) \\ &\quad - \frac{1}{\mathcal{RRHM}_1(\mathcal{G})} \sum_{uv \in E(\mathcal{G})} [(\mathcal{RR}(u) + \mathcal{RR}(v))^2 \times \log((\mathcal{RR}(u) + \mathcal{RR}(v))^2)] \end{aligned}$$

$$= \log(\mathcal{RRHM}_1(\mathcal{G})) - \frac{1}{\mathcal{RRHM}_1(\mathcal{G})} [(2p + 2q + 4pq) \times 64 \times \log 64 + (8p + 8q + 8pq + 8) \times 49 \times \log 49 + (4p + 4q + 8) \times 64 \times \log 64 + (14p + 14q + 28pq) \times 36 \times \log 36 + (4p + 4q + 4pq + 4) \times 25 \times \log 25]. \quad (29)$$

4.4. Second reduced reverse hyper Zagreb entropy.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = (\mathcal{RR}(u) \times \mathcal{RR}(v))^2$ and $\mathcal{RRHM}_2(\mathcal{G}) = 3904p + 3904q + 4464pq + 3344$, then the second reduced reverse hyper Zagreb entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{RRHM}_2(\mathcal{G})} &= \log(\mathcal{RRHM}_2(\mathcal{G})) \\ &\quad - \frac{1}{\mathcal{RRHM}_2(\mathcal{G})} \sum_{uv \in E(\mathcal{G})} [(\mathcal{RR}(u) \times \mathcal{RR}(v))^2 \times \log(\mathcal{RR}(u) \times \mathcal{RR}(v))^2] \\ &= \log(\mathcal{RRHM}_2(\mathcal{G})) - \frac{1}{\mathcal{RRHM}_2(\mathcal{G})} [(2p + 2q + 4pq) \times 225 \times \log 225 + (8p + 8q + 8pq + 8) \times 144 \times \log 144 + (4p + 4q + 8) \times 256 \times \log 256 + (14p + 14q + 28pq) \times 81 \times \log 81 + (4p + 4q + 4pq + 4) \times 36 \times \log 36]. \end{aligned} \quad (30)$$

4.5. Reduced reverse forgotten entropy.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \mathcal{RR}(u)^2 + \mathcal{RR}(v)^2$ and $\mathcal{RRF}(\mathcal{G}) = 700p + 700q + 892pq + 308$, then the reduced reverse forgotten entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{RRF}(\mathcal{G})} &= \log(\mathcal{RRF}(\mathcal{G})) \\ &\quad - \frac{1}{\mathcal{RRF}(\mathcal{G})} \sum_{uv \in E(\mathcal{G})} [(\mathcal{RR}(u)^2 + \mathcal{RR}(v)^2) \times \log(\mathcal{RR}(u)^2 + \mathcal{RR}(v)^2)] \\ &= \log(\mathcal{RRF}(\mathcal{G})) - \frac{1}{\mathcal{RRF}(\mathcal{G})} [(2p + 2q + 4pq) \times 34 \times \log 34 + (8p + 8q + 8pq + 8) \times 25 \times \log 25 + (4p + 4q + 8) \times 32 \times \log 32 + (14p + 14q + 28pq) \times 18 \times \log 18 + (4p + 4q + 4pq + 4) \times 13 \times \log 13]. \end{aligned} \quad (31)$$

4.6. Reduced reverse atom-bond connectivity (**ABC**) entropy.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \sqrt{\frac{\mathcal{RR}(u) + \mathcal{RR}(v) - 2}{\mathcal{RR}(u) \times \mathcal{RR}(v)}}$ and $\mathcal{RRABC}(\mathcal{G}) = 21.0408p + 21.0408q + 29.19pq + 12.89$, then the reduced reverse atom-bond connectivity (**ABC**) entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{RRABC}(\mathcal{G})} &= \log(\mathcal{RRABC}(\mathcal{G})) \\ &\quad - \frac{1}{\mathcal{RRABC}(\mathcal{G})} \sum_{uv \in E(\mathcal{G})} \left[\sqrt{\frac{\mathcal{RR}(u) + \mathcal{RR}(v) - 2}{\mathcal{RR}(u) \times \mathcal{RR}(v)}} \right. \\ &\quad \left. \times \log \left(\sqrt{\frac{\mathcal{RR}(u) + \mathcal{RR}(v) - 2}{\mathcal{RR}(u) \times \mathcal{RR}(v)}} \right) \right] \\ &= \log(\mathcal{RRABC}(\mathcal{G})) - \frac{1}{\mathcal{RRABC}(\mathcal{G})} [(2p + 2q + 4pq) \times \sqrt{\frac{2}{5}} \times \log \left(\sqrt{\frac{2}{5}} \right) \\ &\quad + (8p + 8q + 8pq + 8) \times \sqrt{\frac{5}{12}} \times \log \left(\sqrt{\frac{5}{12}} \right) + (4p + 4q + 8) \times \sqrt{\frac{3}{8}} \times \log \left(\sqrt{\frac{3}{8}} \right)] \end{aligned}$$

$$+ (14p + 14q + 28pq) \times \sqrt{\frac{4}{9}} \times \log \left(\sqrt{\frac{4}{9}} \right) + (4p + 4q + 4pq + 4) \times \sqrt{\frac{1}{2}} \times \log \left(\sqrt{\frac{1}{2}} \right). \quad (32)$$

4.7. Reduced reverse geometric-arithmetic (GA) entropy.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \frac{2\sqrt{\mathcal{RR}(u) \times \mathcal{RR}(v)}}{\mathcal{RR}(u) + \mathcal{RR}(v)}$ and $\mathcal{RRGA}(\mathcal{G}) = 31.7736p + 31.7736q + 43.7101pq + 19.8371$, then the reduced reverse geometric-arithmetic (GA) entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{RRGA}(\mathcal{G})} &= \log(\mathcal{RRGA}(\mathcal{G})) \\ &\quad - \frac{1}{\mathcal{RRGA}(\mathcal{G})} \sum_{uv \in E(\mathcal{G})} \left[\left(\frac{2\sqrt{\mathcal{RR}(u) \times \mathcal{RR}(v)}}{\mathcal{RR}(u) + \mathcal{RR}(v)} \right) \times \log \left(\frac{2\sqrt{\mathcal{RR}(u) \times \mathcal{RR}(v)}}{\mathcal{RR}(u) + \mathcal{RR}(v)} \right) \right] \\ &= \log(\mathcal{RRGA}(\mathcal{G})) - \frac{1}{\mathcal{RRGA}(\mathcal{G})} \left[(2p + 2q + 4pq) \times \frac{\sqrt{15}}{4} \times \log \left(\frac{\sqrt{15}}{4} \right) \right. \\ &\quad \left. + (8p + 8q + 8pq + 8) \times \frac{4\sqrt{3}}{7} \times \log \left(\frac{4\sqrt{3}}{7} \right) + (4p + 4q + 4pq + 4) \times \frac{2\sqrt{6}}{5} \times \right. \\ &\quad \left. \log \left(\frac{2\sqrt{6}}{5} \right) \right]. \quad (33) \end{aligned}$$

4.8. Reduced reverse redefined first Zagreb entropy.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \frac{\mathcal{RR}(u) + \mathcal{RR}(v)}{\mathcal{RR}(u) \times \mathcal{RR}(v)}$ and $\mathcal{RR}[ReZ_1(\mathcal{G})] = 20.40p + 20.40q + 28.80pq + 12$, then the reduced reverse redefined first Zagreb entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{RR}[ReZ_1(\mathcal{G})]} &= \log(\mathcal{RR}[ReZ_1(\mathcal{G})]) \\ &\quad - \frac{1}{\mathcal{RR}[ReZ_1(\mathcal{G})]} \sum_{uv \in E(\mathcal{G})} \left[\left(\frac{\mathcal{RR}(u) + \mathcal{RR}(v)}{\mathcal{RR}(u) \times \mathcal{RR}(v)} \right) \times \log \left(\frac{\mathcal{RR}(u) + \mathcal{RR}(v)}{\mathcal{RR}(u) \times \mathcal{RR}(v)} \right) \right] \\ &= \log(\mathcal{RR}[ReZ_1(\mathcal{G})]) - \frac{1}{\mathcal{RR}[ReZ_1(\mathcal{G})]} \left[(2p + 2q + 4pq) \times \frac{8}{15} \times \log \left(\frac{8}{15} \right) \right. \\ &\quad \left. + (8p + 8q + 8pq + 8) \times \frac{7}{12} \times \log \left(\frac{7}{12} \right) + (4p + 4q + 8) \times \frac{1}{2} \times \log \left(\frac{1}{2} \right) \right. \\ &\quad \left. + (14p + 14q + 28pq) \times \frac{2}{3} \times \log \left(\frac{2}{3} \right) + (4p + 4q + 4pq + 4) \times \frac{5}{6} \times \right. \\ &\quad \left. \log \left(\frac{5}{6} \right) \right]. \quad (34) \end{aligned}$$

4.9. Reduced reverse redefined second Zagreb entropy.

If $f(\mathcal{RR}(u), \mathcal{RR}(v)) = \frac{\mathcal{RR}(u) \times \mathcal{RR}(v)}{\mathcal{RR}(u) + \mathcal{RR}(v)}$ and $\mathcal{RR}[ReZ_2(\mathcal{G})] = 51.26p + 51.26q + 68.01pq + 34.51$, then the reduced reverse redefined second Zagreb entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{RR}[ReZ_2(\mathcal{G})]} &= \log(\mathcal{RR}[ReZ_2(\mathcal{G})]) \\ &\quad - \frac{1}{\mathcal{RR}[ReZ_2(\mathcal{G})]} \sum_{uv \in E(\mathcal{G})} \left[\left(\frac{\mathcal{RR}(u) \times \mathcal{RR}(v)}{\mathcal{RR}(u) + \mathcal{RR}(v)} \right) \times \log \left(\frac{\mathcal{RR}(u) \times \mathcal{RR}(v)}{\mathcal{RR}(u) + \mathcal{RR}(v)} \right) \right] \\ &= \log(\mathcal{RR}[ReZ_2(\mathcal{G})]) - \frac{1}{\mathcal{RR}[ReZ_2(\mathcal{G})]} \left[(2p + 2q + 4pq) \times \frac{15}{8} \times \log \left(\frac{15}{8} \right) \right. \\ &\quad \left. + (8p + 8q + 8pq + 8) \times \frac{12}{7} \times \log \left(\frac{12}{7} \right) + (4p + 4q + 8) \times 2 \times \log 2 \right] \end{aligned}$$

$$+ (14p + 14q + 28pq) \times \frac{3}{2} \times \log\left(\frac{3}{2}\right) + (4p + 4q + 4pq + 4) \times \frac{6}{5} \times \log\left(\frac{6}{5}\right)]. \quad (35)$$

4.10. Reduced reverse redefined third Zagreb entropy.

If $f(\mathcal{R}\mathcal{R}(u), \mathcal{R}\mathcal{R}(v)) = (\mathcal{R}\mathcal{R}(u) + \mathcal{R}\mathcal{R}(v))(\mathcal{R}\mathcal{R}(u) \times \mathcal{R}\mathcal{R}(v))$ and $\mathcal{R}\mathcal{R}[ReZ_3(G)] = 2300p + 2300q + 2784pq + 1816$, then the reduced reverse redefined third Zagreb entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{R}\mathcal{R}[ReZ_3(G)]} &= \log(\mathcal{R}\mathcal{R}[ReZ_3(G)]) - \frac{1}{\mathcal{R}\mathcal{R}[ReZ_3(G)]} \times \sum_{uv \in E(G)} [(\mathcal{R}\mathcal{R}(u) + \mathcal{R}\mathcal{R}(v)) \\ &\quad (\mathcal{R}\mathcal{R}(u) \times \mathcal{R}\mathcal{R}(v)) \times \log((\mathcal{R}\mathcal{R}(u) + \mathcal{R}\mathcal{R}(v))(\mathcal{R}\mathcal{R}(u) \times \mathcal{R}\mathcal{R}(v)))] \\ &= \log(\mathcal{R}\mathcal{R}[ReZ_3(G)]) - \frac{1}{\mathcal{R}\mathcal{R}[ReZ_3(G)]} [(2p + 2q + 4pq) \times 120 \times \log 120 \\ &\quad + (8p + 8q + 8pq + 8) \times 84 \times \log 84 + (4p + 4q + 8) \times 128 \times \log 128 \\ &\quad + (14p + 14q + 28pq) \times 54 \times \log 54 + (4p + 4q + 4pq + 4) \times 30 \times \log 30]. \end{aligned} \quad (36)$$

4.11. Reduced reverse generalized Zagreb entropy.

If $f(\mathcal{R}\mathcal{R}(u), \mathcal{R}\mathcal{R}(v)) = \mathcal{R}\mathcal{R}(u)^r \times \mathcal{R}\mathcal{R}(v)^s + \mathcal{R}\mathcal{R}(u)^s \times \mathcal{R}\mathcal{R}(v)^r$ and $\mathcal{R}\mathcal{R}[M_{r,s}(G)] = (2p + 2q + 4pq)(5^r \times 3^s + 5^s \times 3^r) + (8p + 8q + 8pq + 8)(4^r \times 3^s + 4^s \times 3^r) + (8p + 8q + 16)(4^{r+s}) + (28p + 28q + 56pq)(3^{r+s}) + (4p + 4q + 4pq + 4)(3^r \times 2^s + 3^s \times 2^r)$,

then the reduced reverse generalized Zagreb entropy is

$$\begin{aligned} \mathbb{E}_{\mathcal{R}\mathcal{R}[M_{r,s}(G)]} &= \log(\mathcal{R}\mathcal{R}[M_{r,s}(G)]) - \frac{1}{\mathcal{R}\mathcal{R}[M_{r,s}(G)]} \sum_{uv \in E(G)} [(\mathcal{R}\mathcal{R}(u)^r \times \mathcal{R}\mathcal{R}(v)^s \\ &\quad + \mathcal{R}\mathcal{R}(u)^s \times \mathcal{R}\mathcal{R}(v)^r) \times \log(\mathcal{R}\mathcal{R}(u)^r \times \mathcal{R}\mathcal{R}(v)^s + \mathcal{R}\mathcal{R}(u)^s \times \mathcal{R}\mathcal{R}(v)^r)] \\ &= \log(\mathcal{R}\mathcal{R}[M_{r,s}(G)]) - \frac{1}{\mathcal{R}\mathcal{R}[M_{r,s}(G)]} [(2p + 2q + 4pq) \times (5^r \times 3^s + 5^s \times 3^r) \\ &\quad \times \log(5^r \times 3^s + 5^s \times 3^r) + (8p + 8q + 8pq + 8) \times (4^r \times 3^s + 4^s \times 3^r) \\ &\quad \times \log(4^r \times 3^s + 4^s \times 3^r) + (8p + 8q + 16) \times (4^{r+s}) \times \log(2 \times 4^{r+s}) \\ &\quad + (28p + 28q + 56pq) \times (3^{r+s}) \times \log(2 \times 3^{r+s}) + (4p + 4q + 4pq + 4) \\ &\quad \times (3^r \times 2^s + 3^s \times 2^r) \times \log(3^r \times 2^s + 3^s \times 2^r)]. \end{aligned} \quad (37)$$

Tables 5 and 6 provide the values of the entropy measures discussed above for specific values of p and q with $p = q = 1, 2, \dots, 20$. Further, Figure 3 gives the graphical interpretation of the entropies for these values of p and q .

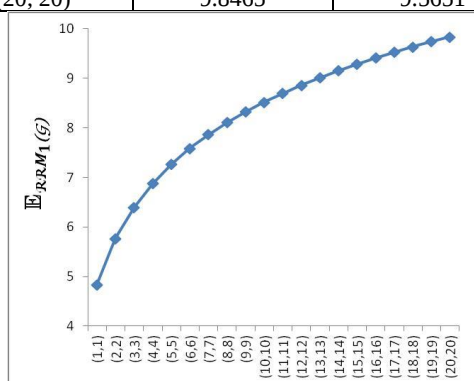
Table 5. Numerical behaviour of entropy measures of $G = TCNB(p, q)$ for some specific values of p and q with $p = q$.

(p, q)	$\mathbb{E}_{RRM_1(G)}$	$\mathbb{E}_{RRM_2(G)}$	$\mathbb{E}_{RRHM_1(G)}$	$\mathbb{E}_{RRHM_2(G)}$	$\mathbb{E}_{RRF(G)}$
(1, 1)	4.8417	4.812	4.8114	4.7021	4.4957
(2, 2)	5.7716	5.7457	5.744	5.6439	5.7801
(3, 3)	6.4016	6.3776	6.3754	6.281	6.3078
(4, 4)	6.8793	6.8565	6.854	6.7633	6.8108
(5, 5)	7.2644	7.2423	7.2396	7.1515	7.2091
(6, 6)	7.587	7.5655	7.5627	7.4765	7.5396
(7, 7)	7.8647	7.8436	7.8407	7.7559	7.8223
(8, 8)	8.1085	8.0876	8.0847	8.001	8.0695
(9, 9)	8.3257	8.3051	8.3021	8.2193	8.2891
(10, 10)	8.5216	8.5012	8.4981	8.4162	8.4869

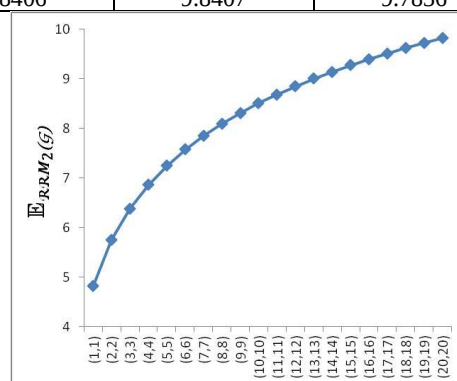
(p, q)	$\mathbb{E}_{RRM_1}(\mathcal{G})$	$\mathbb{E}_{RRM_2}(\mathcal{G})$	$\mathbb{E}_{RRHM_1}(\mathcal{G})$	$\mathbb{E}_{RRHM_2}(\mathcal{G})$	$\mathbb{E}_{RRF}(\mathcal{G})$
(11, 11)	8.7	8.6798	8.6767	8.5953	8.6666
(12, 12)	8.8638	8.8437	8.8406	8.7597	8.8315
(13, 13)	9.0152	8.9952	8.992	8.9117	8.9837
(14, 14)	9.1559	9.136	9.1328	9.0529	9.1251
(15, 15)	9.2873	9.2676	9.2644	9.1848	9.2571
(16, 16)	9.4107	9.391	9.3878	9.3085	9.3809
(17, 17)	9.5269	9.5073	9.504	9.425	9.4975
(18, 18)	9.6367	9.6171	9.6139	9.5351	9.6076
(19, 19)	9.7407	9.7213	9.718	9.6394	9.712
(20, 20)	9.8397	9.8202	9.817	9.7386	9.8112

Table 6. Numerical behaviour of entropy measures of $\mathcal{G} = TCNB(p, q)$ for some specific values of p and q with $p = q$.

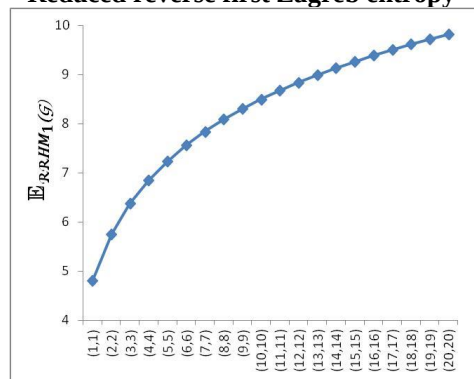
(p, q)	$\mathbb{E}_{RRABC}(\mathcal{G})$	$\mathbb{E}_{RRGA}(\mathcal{G})$	$\mathbb{E}_{RR[ReZ_1]}(\mathcal{G})$	$\mathbb{E}_{RR[ReZ_2]}(\mathcal{G})$	$\mathbb{E}_{RR[ReZ_3]}(\mathcal{G})$
(1, 1)	4.8513	4.4744	4.8413	4.8417	4.7641
(2, 2)	5.7801	5.4452	5.7719	5.772	5.7012
(3, 3)	6.4096	6.0923	6.4021	6.4022	6.3353
(4, 4)	6.8871	6.5794	6.8799	6.8801	6.8155
(5, 5)	7.2719	6.9704	7.2651	7.2652	7.2022
(6, 6)	7.5944	7.2972	7.5878	7.5879	7.5261
(7, 7)	7.872	7.5778	7.8655	7.8656	7.8047
(8, 8)	8.1157	7.8239	8.1093	8.1094	8.0491
(9, 9)	8.3329	8.0429	8.3265	8.3267	8.2669
(10, 10)	8.5287	8.2403	8.5224	8.5226	8.4633
(11, 11)	8.7071	8.4199	8.7008	8.701	8.6421
(12, 12)	8.8708	8.5847	8.8646	8.8648	8.8062
(13, 13)	9.0222	8.7369	9.016	9.0162	8.9579
(14, 14)	9.1629	8.8784	9.1567	9.1569	9.0989
(15, 15)	9.2943	9.0105	9.2882	9.2884	9.2305
(16, 16)	9.4176	9.1344	9.4116	9.4117	9.3541
(17, 17)	9.5338	9.2511	9.5277	9.5279	9.4704
(18, 18)	9.6436	9.3613	9.6375	9.6377	9.5804
(19, 19)	9.7476	9.4658	9.7416	9.7418	9.6846
(20, 20)	9.8465	9.5651	9.8406	9.8407	9.7836



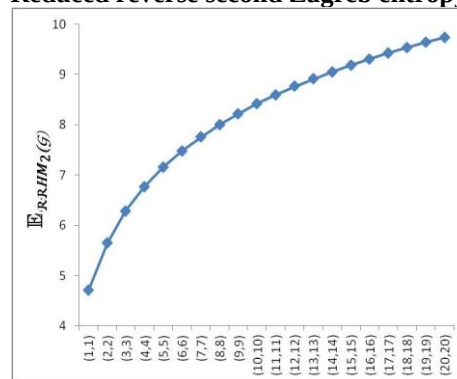
Reduced reverse first Zagreb entropy



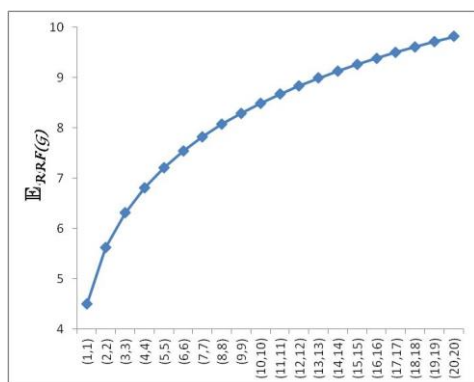
Reduced reverse second Zagreb entropy



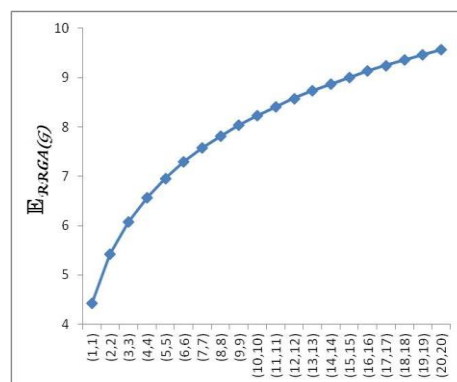
Reduced reverse first hyper Zagreb entropy



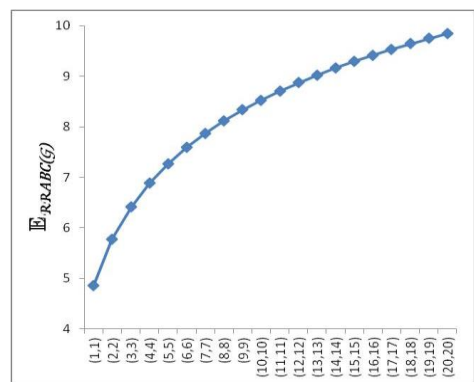
Reduced reverse second hyper Zagreb entropy



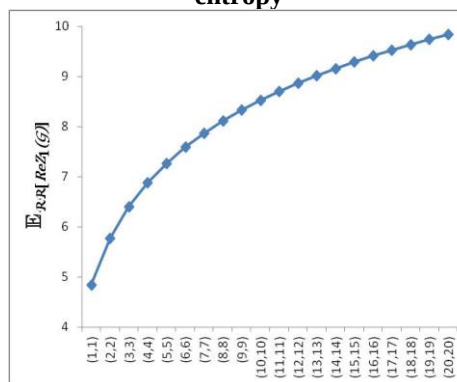
Reduced reverse forgotten entropy



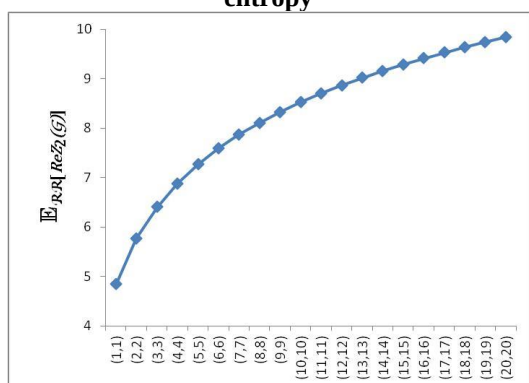
Reduced reverse geometric-arithmetic Zagreb entropy



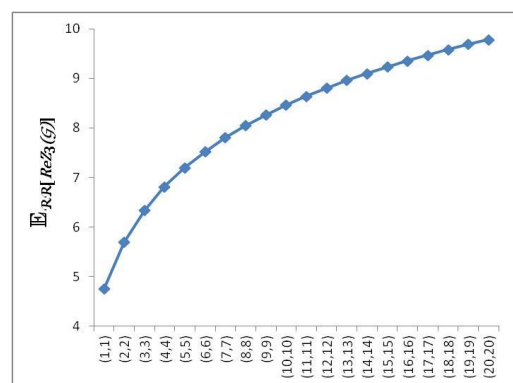
Reduced reverse first atom-bond connectivity entropy



Reduced reverse redefined first Zagreb entropy



Reduced reverse redefined second Zagreb entropy



Reduced reverse redefined third Zagreb entropy

Figure 3. Graphical representation of reduced reverse degree-based entropy of $G = TCNB(p, q)$.

5. Regression Analysis

Regression is a statistical technique that examines the relationship between the dependent variable, also known as the response variable, and the independent variable, also referred to as the predictor variable. In this study, we use a logarithmic regression model to examine the relationship between the various reduced reverse topological indices (*TIs*) and their corresponding entropy measures (*E*s) of $TCNB(p, q)$ for $1 \leq p, q \leq 20$. The most general form of a logarithmic regression model is

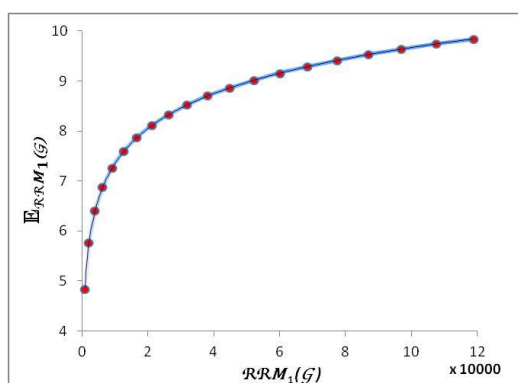
$$y = a \times \ln(x) + b,$$

where y is the dependent variable, x is the independent variable, $\ln$ is the natural logarithm, a is the regression coefficient, and b is the regression constant. In this context, we consider the dependent variable as an entropy measure and the independent variable as a topological index. The analysis includes statistical measures such as the squared correlation

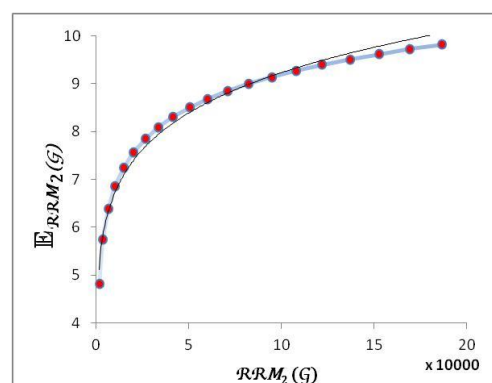
coefficient (R^2), the sum of square error (SSE), root mean squared error ($RMSE$), F -Value, and Significance F .

Table 7. Statistical measures of reduced reverse topological indices vs. entropy measures of $G = TCNB(p, q)$.

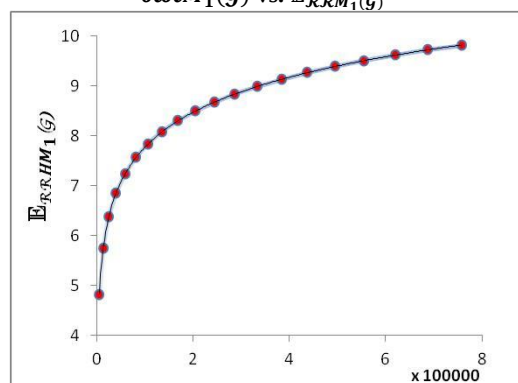
Data	Model	R^2	SSE	$RMSE$	F	$Sig. F$
$RRM_1(G)$ vs. $E_{RRM_1}(G)$	$y = 1.0059 \times \ln(x) - 1.9111$	1	0.000218	0.003481	3088693	1.44×10^{-48}
$RRM_2(G)$ vs. $E_{RRM_2}(G)$	$y = 1.0142 \times \ln(x) - 2.4813$	1	0.001218	0.008226	554889	7.37×10^{-42}
$RRHM_1(G)$ vs. $E_{RRHM_1}(G)$	$y = 1.0136 \times \ln(x) - 3.8981$	1	0.001106	0.007840	610343	3.13×10^{-42}
$RRHM_2(G)$ vs. $E_{RRHM_2}(G)$	$y = 1.0361 \times \ln(x) - 5.2457$	1	0.000373	0.019305	101788	3.13×10^{-35}
$RRF(G)$ vs. $E_{RRF}(G)$	$y = 1.0445 \times \ln(x) - 3.5889$	1	0.030014	0.040834	24386	1.2×10^{-29}
$RRAB(G)$ vs. $E_{RRAB}(G)$	$y = 0.9868 \times \ln(x) + 0.9289$	1	0.00325	0.13437	207855.6	5.08×10^{-38}
$RRGA(G)$ vs. $E_{RRGA}(G)$	$y = 1.0153 \times \ln(x) - 0.4164$	1	0.001567	0.00933	442689.3	5.63×10^{-41}
$RR[ReZ_1(G)]$ vs. $E_{RR[ReZ_1](G)}$	$y = 0.9968 \times \ln(x) + 0.4476$	1	0.000071	0.001991	9439104	6.19×10^{-53}
$RR[ReZ_2(G)]$ vs. $E_{RR[ReZ_2](G)}$	$y = 1.0060 \times \ln(x) - 0.5029$	1	0.000233	0.003597	2892583	2.59×10^{-48}
$RR[ReZ_3(G)]$ vs. $E_{RR[ReZ_3](G)}$	$y = 1.0238 \times \ln(x) - 4.5410$	1	0.003811	0.013293	213361.1	4.01×10^{-38}



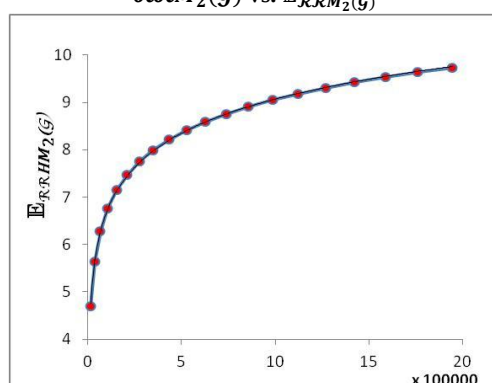
$RRM_1(G)$ vs. $E_{RRM_1}(G)$



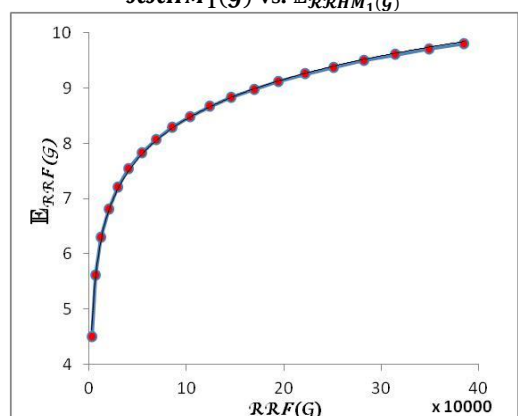
$RRM_2(G)$ vs. $E_{RRM_2}(G)$



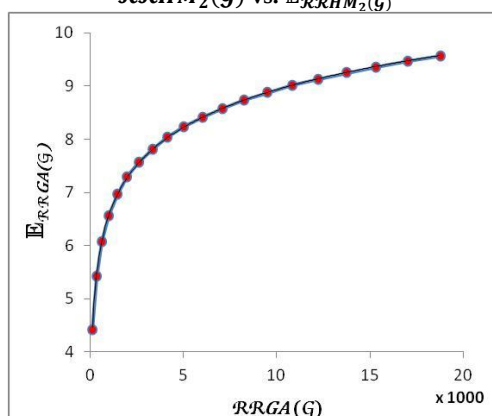
$RRHM_1(G)$ vs. $E_{RRHM_1}(G)$



$RRHM_2(G)$ vs. $E_{RRHM_2}(G)$



$RRF(G)$ vs. $E_{RRF}(G)$



$RRGA(G)$ vs. $E_{RRGA}(G)$

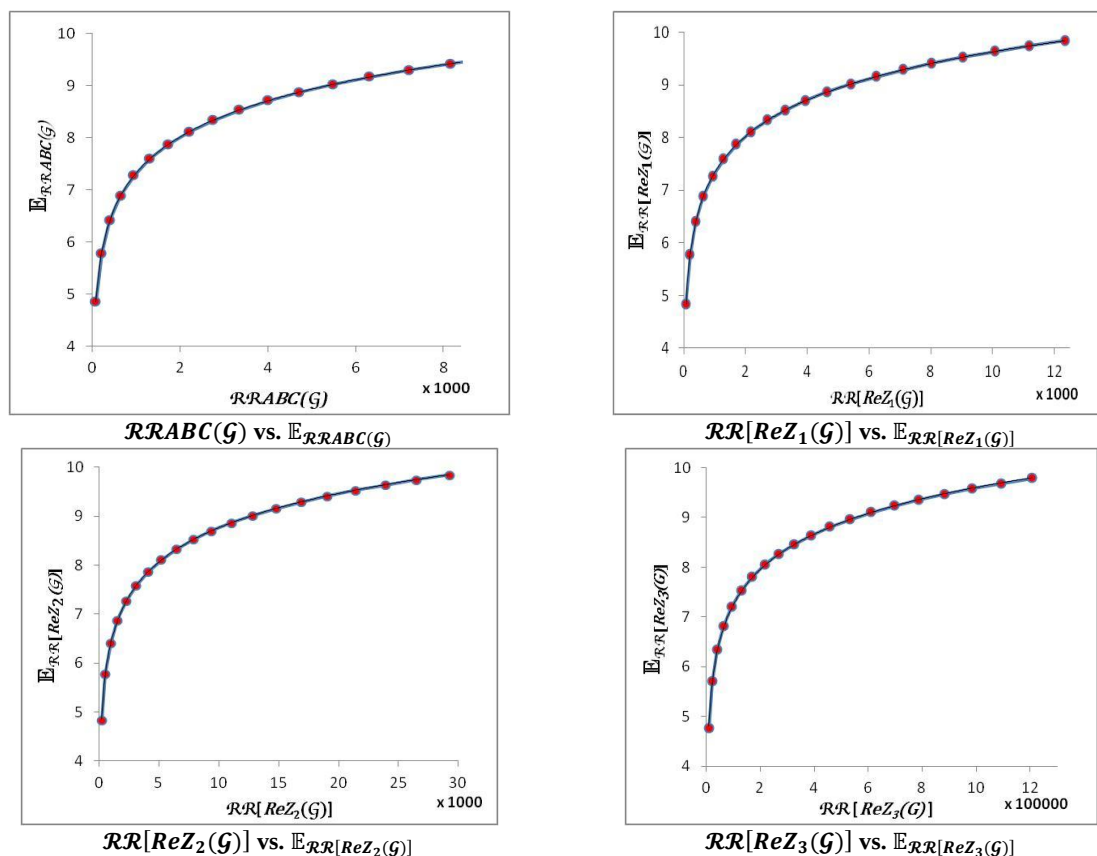


Figure 4. Comparison of the reduced reverse topological indices and their corresponding entropy measures of $G = TCNB(p, q)$.

The logarithmic regression curve fitting statistical values of the earlier discussed reduced reverse topological indices versus corresponding entropy measures for the $TCNB(p, q)$ are shown in Table 7.

6. Numerical and Graphical Discussion

In this section, we have made a comprehensive analysis of various reduced reverse vertex degree-based topological indices and their corresponding entropies of the Tetracyanobenzene metal organic framework $TCNB(p, q)$. Based on the regression analysis carried out in the previous section, with reference to the values of the aforesaid indices for different values of p and q are tabulated in Tables 3 and 4, while the corresponding entropy values are tabulated in Tables 5 and 6.

An increase in the values of p and q ensures a corresponding increase in each of the discussed indices and entropies. This trend is observed in the graphs in Figures 2 and 3. Consistent trends are observed between the considered sets of indices and entropies. Of all the indices, the reduced reverse atom-bond connectivity index $RRM_3(G)$ takes the least value, whereas the second reduced reverse hyper-Zagreb index $RRHM_2(G)$ takes the greatest value. Similarly, of all the entropy measures, the reduced reverse geometric-arithmetic entropy $E_{RGA}(G)$ takes the least value, whereas the reduced reverse atom-bond connectivity entropy $E_{RABC}(G)$ takes the greatest value. Unfortunately, it is not possible to determine the entropy value for the third reduced reverse Zagreb index due to encountering an undefined value $\log 0$ when the adjacent vertices have the same degree. Further, we made the comparison of topological indices with their entropy measures by a logarithmic regression model, which is shown in Table 7. In each regression model, the value of R^2 is identically equal to 1, and the

values of SSE and $RMSE$ are very low. Additionally, the values of F are found to be very large, and the significance F -values are quite small. These results indicate a strong correlation between the discussed indices and their corresponding entropies, suggesting that the differences in group means are substantially greater than the variability within each group. Consequently, the observed differences are unlikely to be due to chance alone.

7. Conclusion

In this article, we derive the expressions for the closed forms of various reduced reverse vertex degree-based topological indices and the corresponding entropy measures of the Tetracyanobenzene metal-organic frameworks. Further, we have made a graphical and comparative analysis of these indices and the entropy measures by computing them for different values of p and q . The analysis of the existing relationships between these indices, as well as entropy measures and the topological properties of the structure, is conducted using a logarithmic regression model. Based on the analysis, it is concluded that these indices and entropy measures are significantly correlated.

8. Future Work

As seen in literature, topological indices are found to have strong correlation with many of the structural, physical, and chemical properties of MOFs. They play a significant role in understanding how the MOF structures influence their properties. For example, Zagreb indices are seen to correlate with the stability of MOFs. Similarly, the Wiener index is useful in predicting the porosity of these structures.

Taking this direction, further computational research may shed light on the significance of the topological indices discussed in this study in predicting the physicochemical properties of broader classes of MOFs by incorporating real-world chemical data for validation. Integrating these indices with machine learning could ensure improved computational efficiency, especially when dealing with large-scale datasets.

Author Contributions

Conceptualization, S.C.K., S.D., N.N.S., H.S., and S.A.S.; methodology, S.C.K., S.D., N.N.S., H.S., and S.A.S.; writing—original draft preparation, S.C.K., S.D., N.N.S., H.S., and S.A.S.; All authors have read and agreed to the published version of the manuscript.

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The data used to support the findings of this study are included within the article.

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Conflicts of Interest

The authors declare no conflict of interest.

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