

Research Article

On Curvilinear Regression Analysis via Newly Proposed Entropies for Some Benzene Models

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To avoid exorbitant and extensive laboratory experiments, QSPR analysis, based on topological descriptors, is a very constructive statistical approach for analyzing the numerous physical and chemical properties of compounds. Therefore, we presented some new entropy measures which are based on the sum of the neighborhood degree of the vertices. Firstly, we made the partition of the edges of benzene derivatives which are based on the degree sum of neighboring vertices and then computed the neighborhood version of entropies. Secondly, we made use of the software SPSS for developing a correlation between newly introduced entropies and the physicochemical properties of benzene derivatives. Our obtained results demonstrated that the critical temperature ($\mathcal{E}\mathcal{T}$), critical pressure ($\mathcal{E}\mathcal{P}$), and critical volume ($\mathcal{E}\mathcal{V}$) can be predicted through fifth geometric arithmetic entropy, second SK entropy, and fifth ND entropy, respectively. Other remaining physical characteristics include Gibb's energy ($q\mathcal{E}$), $\log(P)$, molar refractivity ($\mathcal{M}\mathcal{R}$), and Henry's law ($\mathcal{H}\mathcal{L}$) that can be predicted by using sixth ND entropy.

1. Introduction

In chemistry, models are classified into two types. The first type of modeling is based on the quantum-chemical method and theoretically identical models derived from statistical mechanics. The second type consists of chemical thinking, which compares related systems. According to the core principle of chemistry, all the features of matter correlate with its molecular structure, and thus, molecules with similar structures have similar properties. This has resulted in several empirical approaches such as SAR, SPC, QSPR, and QSAR [1, 2].

The identical factor of all these methods is the correlation between physicochemical properties and molecular descriptors. There are numerous descriptors to utilize [3], but one family of descriptors has been demonstrated exceptionally basic and valuable in foreseeing multiple molecular properties. These are known as topological indices ($\mathcal{T}\mathcal{I}\mathcal{S}$).

Topological indices ($\mathcal{T}\mathcal{I}\mathcal{S}$) are numerical parameters that are correlated with a graph and help identify its topology. There are three types of $\mathcal{T}\mathcal{I}\mathcal{S}$: degree-based $\mathcal{T}\mathcal{I}\mathcal{S}$, spectrum-based $\mathcal{T}\mathcal{I}\mathcal{S}$, and distance-based $\mathcal{T}\mathcal{I}\mathcal{S}$ [4, 5]. Degree-based $\mathcal{T}\mathcal{I}\mathcal{S}$, which are defined in terms of the degrees of the vertices of a graph, are one of the most studied $\mathcal{T}\mathcal{I}\mathcal{S}$ used in mathematical chemistry [6]. Imran et al. [7] discuss the topological properties of symmetric chemical structures. Zou et al. [8] computed topological indices for polyphenylene. Recently, some neighborhood versions of $\mathcal{T}\mathcal{I}\mathcal{S}$ have also been introduced [9, 10]. Zhang et al. [11–13] discuss the topological indices of generalized bridge molecular graphs, carbon nanotubes, and the product of chemical graphs.

The idea of entropy first appeared in thermodynamics in the nineteenth century, when it was closely linked to the heat flow and a key component of the second law of thermodynamics. Subsequently, statistical mechanics used the

notion to illuminate thermodynamics physically. Leading physicists such as Boltzmann and Gibbs [14, 15], who employed entropy as a measure of the disorder of the massive dynamical system underlying molecule collections, were responsible for this. Fisher employed similar notions in the establishment of the foundations of theoretical statistics in 1920 [16]. In the 1950s, Kullback and Leibler [17] developed this concept further. Zhang et al. [18–20] provided the physical analysis of heat for the formation and entropy of ceria oxide.

Claude Shannon, a mathematician and electrical engineer who worked at Bell Labs in New Jersey in the midtwentieth century, identified the link between entropy and information content [21]. The concept formed a key element of the emerging field of information theory at that time. Afterward, in the 1950s, Jaynes explained the explicit association between Shannon's entropy and that of statistical mechanics in a series of excellent works [22, 23]. Since then, information theory has found applications in a variety of fields, including networking analysis, mathematical statistics, complexity theory, and financial mathematics.

We made a bibliometric analysis grounded on the Scopus database <https://www.scopus.com>. This analysis is based upon 986 research articles with entropy and graph entropy [24–26] as key factors. The percentage of publications in different subjects is shown in Figure 1.

We made a bibliometric analysis of the research conducted in different countries on the concept of entropy in Figure 2.

In recent times, another approach which is a bit different in the literature, namely, using the concept of Shannon's entropy in terms of topological indices was introduced by Manzoor et al. in [27]. Continuing their work, they also introduced eccentricity-based graph entropies [28, 29] and bond additive graph entropies [30]. In this paper, the present authors formulated some new graph entropies, namely, neighborhood versions of graph entropies. The graph entropy is represented in the following formula:

$$\mathfrak{G}_i(\mathfrak{B}) = - \sum_{\mathbf{u}'\mathbf{b}' \in \mathfrak{C}(\mathfrak{B})} \frac{\mathbb{I}(\mathbf{u}'\mathbf{b}')}{\sum_{\mathbf{u}\mathbf{v} \in \mathfrak{C}(\mathfrak{B})} \mathbb{I}(\mathbf{u}\mathbf{v})} \log_2 \left[\frac{\mathbb{I}(\mathbf{u}'\mathbf{b}')}{\sum_{\mathbf{u}\mathbf{v} \in \mathfrak{C}(\mathfrak{B})} \mathbb{I}(\mathbf{u}\mathbf{v})} \right], \quad (1)$$

where $\mathcal{V}(\mathfrak{B})$ is the vertex set, $\mathfrak{C}(\mathfrak{B})$ is the edge set, and $\mathbb{I}(\mathbf{u}\mathbf{v})$ is the edge weight of the edge $(\mathbf{u}\mathbf{v})$.

(i) Neighborhood version of forgotten entropy

If $\mathbb{I}(\mathbf{u}\mathbf{v}) = \mathfrak{A}(\mathbf{u})^2 + \mathfrak{A}(\mathbf{v})^2$, then

$$\sum_{\mathbf{u}\mathbf{v} \in \mathfrak{C}(\mathfrak{B})} \mathbb{I}(\mathbf{u}\mathbf{v}) = \sum_{\mathbf{u}\mathbf{v} \in \mathfrak{C}(\mathfrak{B})} [\mathfrak{A}(\mathbf{u})^2 + \mathfrak{A}(\mathbf{v})^2] = \mathbb{F}_N^*. \quad (2)$$

So, equation (1) is called the neighborhood version of forgotten entropy.

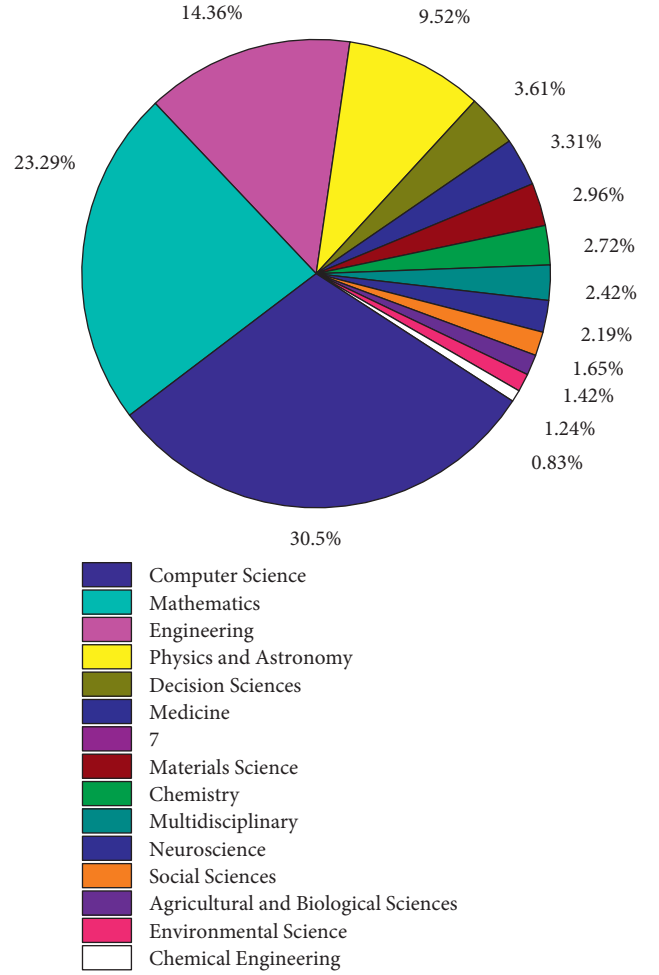


FIGURE 1: Bibliometric analysis of the publications of entropy in various disciplines.

$$\mathfrak{G}_{\mathbb{F}_N^*}(\mathfrak{B}) = \log_2(\mathbb{H}_N^*) - \frac{1}{\mathbb{H}_N^*} \sum_{i=1}^q \sum_{\mathbf{u}\mathbf{v} \in \mathfrak{C}_i(\mathfrak{B})} \cdot [\mathfrak{A}(\mathbf{u})^2 + \mathfrak{A}(\mathbf{v})^2] \log_2 [\mathfrak{A}(\mathbf{u})^2 + \mathfrak{A}(\mathbf{v})^2]. \quad (3)$$

(ii) Neighborhood version of second Zagreb entropy

If $\mathbb{I}(\mathbf{u}\mathbf{v}) = \mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})$, then

$$\sum_{\mathbf{u}\mathbf{v} \in \mathfrak{C}(\mathfrak{B})} \mathbb{I}(\mathbf{u}\mathbf{v}) = \sum_{\mathbf{u}\mathbf{v} \in \mathfrak{C}(\mathfrak{B})} [\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})] = \mathbb{M}_2^*. \quad (4)$$

So, equation (2) is called the neighborhood version of second Zagreb entropy.

$$\mathfrak{G}_{\mathbb{M}_2^*}(\mathfrak{B}) = \log_2(\mathbb{M}_2^*) - \frac{1}{\mathbb{M}_2^*} \sum_{i=1}^q \sum_{\mathbf{u}\mathbf{v} \in \mathfrak{C}_i(\mathfrak{B})} \cdot [\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})] \log_2 [\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})]. \quad (5)$$

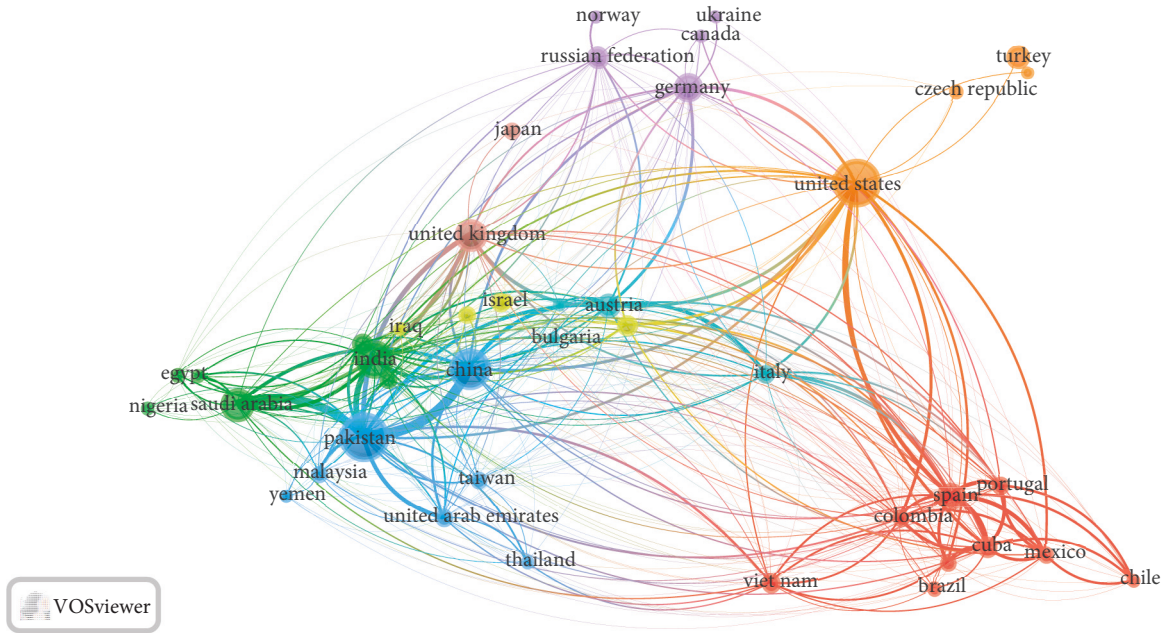


FIGURE 2: Bibliometric analysis of countrywise research based on the topic of entropy. The size of the circles denotes the frequency of articles, and distinct colors are used to signify distinct clusters.

(iii) Neighborhood version of hyper-Zagreb entropy

If $\mathbb{I}(uv) = [\mathfrak{A}(u) + \mathfrak{A}(v)]^2$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} [\mathfrak{A}(u) + \mathfrak{A}(v)]^2 = \text{HM}_N. \quad (6)$$

So, equation (3) is called the neighborhood version of hyper-Zagreb entropy.

$$\mathfrak{G}_{\text{HM}_N}(\mathfrak{B}) = \log_2(\text{HM}_N) - \frac{1}{(\text{HM}_N)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} [\mathfrak{A}(u) + \mathfrak{A}(v)]^2 \log_2 [\mathfrak{A}(u) + \mathfrak{A}(v)]^2. \quad (7)$$

(iv) First ND entropy

If $\mathbb{I}(uv) = \sqrt{\mathfrak{A}(u) \times \mathfrak{A}(v)}$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} [\sqrt{\mathfrak{A}(u) \times \mathfrak{A}(v)}] = \text{ND}_1. \quad (8)$$

So, equation (4) is called the first ND entropy.

$$\mathfrak{G}_{\text{ND}_1}(\mathfrak{B}) = \log_2(\text{ND}_1) - \frac{1}{(\text{ND}_1)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} [\sqrt{\mathfrak{A}(u) \times \mathfrak{A}(v)}] \log_2 [\sqrt{\mathfrak{A}(u) \times \mathfrak{A}(v)}]. \quad (9)$$

(v) Second ND entropy

If $\mathbb{I}(uv) = 1/\sqrt{\mathfrak{A}(u) + \mathfrak{A}(v)}$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{1}{\sqrt{\mathfrak{A}(u) + \mathfrak{A}(v)}} \right] = \text{ND}_2. \quad (10)$$

So, equation (5) is called the second ND entropy.

$$\mathfrak{G}_{\text{ND}_2}(\mathfrak{B}) = \log_2(\text{ND}_2) - \frac{1}{(\text{ND}_2)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \left[\frac{1}{\sqrt{\mathfrak{A}(u) + \mathfrak{A}(v)}} \right] \log_2 \left[\frac{1}{\sqrt{\mathfrak{A}(u) + \mathfrak{A}(v)}} \right]. \quad (11)$$

(vi) Third ND entropy.

If $\mathbb{I}(uv) = [\mathfrak{A}(u) \times \mathfrak{A}(v)][\mathfrak{A}(u) + \mathfrak{A}(v)]$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} [\mathfrak{A}(u) \times \mathfrak{A}(v)] \cdot [\mathfrak{A}(u) + \mathfrak{A}(v)] = \text{ND}_3. \quad (12)$$

So, equation (6) is called the third ND entropy.

$$\mathfrak{G}_{\text{ND}_3}(\mathfrak{B}) = \log_2(\text{ND}_3) - \frac{1}{(\text{ND}_3)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} [\mathfrak{A}(u) \times \mathfrak{A}(v)][\mathfrak{A}(u) + \mathfrak{A}(v)] \log_2 [\mathfrak{A}(u) \times \mathfrak{A}(v)][\mathfrak{A}(u) + \mathfrak{A}(v)]. \quad (13)$$

(vii) Fourth ND entropy.

If $\mathbb{I}(uv) = 1/\sqrt{\mathfrak{A}(u) \times \mathfrak{A}(v)}$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{1}{\sqrt{\mathfrak{A}(u) \times \mathfrak{A}(v)}} \right] = \text{ND}_4. \quad (14)$$

So, equation (7) is called the fourth ND entropy.

$$\begin{aligned} \mathfrak{G}_{\text{ND}_4}(\mathfrak{B}) &= \log_2(\text{ND}_4) - \frac{1}{(\text{ND}_4)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\frac{1}{\sqrt{\mathfrak{A}(u) \times \mathfrak{A}(v)}} \right] \log_2 \left[\frac{1}{\sqrt{\mathfrak{A}(u) \times \mathfrak{A}(v)}} \right]. \end{aligned} \quad (15)$$

(viii) Fifth ND entropy.

If $\mathbb{I}(uv) = \mathfrak{A}(u)/\mathfrak{A}(v) + \mathfrak{A}(v)/\mathfrak{A}(u)$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{\mathfrak{A}(u)}{\mathfrak{A}(v)} + \frac{\mathfrak{A}(v)}{\mathfrak{A}(u)} \right] = \text{ND}_5. \quad (16)$$

So, equation (8) is called the fifth ND entropy.

$$\begin{aligned} \mathfrak{G}_{\text{ND}_5}(\mathfrak{B}) &= \log_2(\text{ND}_5) - \frac{1}{(\text{ND}_5)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\frac{\mathfrak{A}(u)}{\mathfrak{A}(v)} + \frac{\mathfrak{A}(v)}{\mathfrak{A}(u)} \right] \log_2 \left[\frac{\mathfrak{A}(u)}{\mathfrak{A}(v)} + \frac{\mathfrak{A}(v)}{\mathfrak{A}(u)} \right]. \end{aligned} \quad (17)$$

(ix) Sixth ND entropy

If $\mathbb{I}(uv) = \mathfrak{d}(r)\mathfrak{A}(u) + \mathfrak{d}(s)\mathfrak{A}(v)$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} [\mathfrak{d}(r)\mathfrak{A}(u) + \mathfrak{d}(s)\mathfrak{A}(v)] = \text{ND}_6. \quad (18)$$

So, equation (9) is called the sixth ND entropy.

$$\begin{aligned} \mathfrak{G}_{\text{ND}_6}(\mathfrak{B}) &= \log_2(\text{ND}_6) - \frac{1}{(\text{ND}_6)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot [\mathfrak{d}(r)\mathfrak{A}(u) + \mathfrak{d}(s)\mathfrak{A}(v)] \log_2 \\ &\cdot [\mathfrak{d}(r)\mathfrak{A}(u) + \mathfrak{d}(s)\mathfrak{A}(v)]. \end{aligned} \quad (19)$$

(x) Neighborhood version of SK entropy

If $\mathbb{I}(uv) = \mathfrak{A}(u) + \mathfrak{A}(v)/2$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{\mathfrak{A}(u) + \mathfrak{A}(v)}{2} \right] = \text{SK}_N. \quad (20)$$

So, equation (10) is called the neighborhood version of SK entropy.

$$\begin{aligned} \mathfrak{G}_{\text{SK}_N}(\mathfrak{B}) &= \log_2(\text{SK}_N) - \frac{1}{(\text{SK}_N)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\frac{\mathfrak{A}(u) + \mathfrak{A}(v)}{2} \right] \log_2 \left[\frac{\mathfrak{A}(u) + \mathfrak{A}(v)}{2} \right]. \end{aligned} \quad (21)$$

(xi) Neighborhood version of first SK entropy.

If $\mathbb{I}(uv) = \mathfrak{A}(u) \times \mathfrak{A}(v)/2$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{\mathfrak{A}(u) \times \mathfrak{A}(v)}{2} \right] = \text{SK}_{1N}. \quad (22)$$

So, equation (11) is called the neighborhood version of SK entropy.

$$\begin{aligned} \mathfrak{G}_{\text{SK}_{1N}}(\mathfrak{B}) &= \log_2(\text{SK}_{1N}) - \frac{1}{(\text{SK}_{1N})} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\frac{\mathfrak{A}(u) \times \mathfrak{A}(v)}{2} \right] \log_2 \left[\frac{\mathfrak{A}(u) \times \mathfrak{A}(v)}{2} \right]. \end{aligned} \quad (23)$$

(xii) Neighborhood version of second SK entropy.

If $\mathbb{I}(uv) = [\mathfrak{A}(u) + \mathfrak{A}(v)/2]^2$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{\mathfrak{A}(u) + \mathfrak{A}(v)}{2} \right]^2 = \text{SK}_{1N}. \quad (24)$$

So, equation (12) is called the neighborhood version of SK entropy.

$$\begin{aligned} \mathfrak{G}_{\text{SK}_{2N}}(\mathfrak{B}) &= \log_2(\text{SK}_{2N}) - \frac{1}{(\text{SK}_{2N})} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\frac{\mathfrak{A}(u) + \mathfrak{A}(v)}{2} \right]^2 \log_2 \left[\frac{\mathfrak{A}(u) + \mathfrak{A}(v)}{2} \right]^2. \end{aligned} \quad (25)$$

(xiii) Neighborhood version of modified Randi \acute{c} entropy.

If $\mathbb{I}(uv) = 1/\max\{\mathfrak{A}(u), \mathfrak{A}(v)\}$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{1}{\max\{\mathfrak{A}(u), \mathfrak{A}(v)\}} \right] = {}^m\mathbb{R}_N. \quad (26)$$

So, equation (13) is called the neighborhood version of modified Randi \acute{c} entropy.

$$\begin{aligned} \mathfrak{G}_{{}^m\mathbb{R}_N}(\mathfrak{B}) &= \log_2({}^m\mathbb{R}_N) - \frac{1}{({}^m\mathbb{R}_N)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\frac{1}{\max\{\mathfrak{A}(u), \mathfrak{A}(v)\}} \right] \log_2 \left[\frac{1}{\max\{\mathfrak{A}(u), \mathfrak{A}(v)\}} \right]. \end{aligned} \quad (27)$$

(xiv) Neighborhood version of redefined first Zagreb entropy.

If $\mathbb{I}(uv) = \mathfrak{A}(u) + \mathfrak{A}(v)/\mathfrak{A}(u) \times \mathfrak{A}(v)$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{\mathfrak{A}(u) + \mathfrak{A}(v)}{\mathfrak{A}(u) \times \mathfrak{A}(v)} \right] = \mathbb{R}ez_{1N}. \quad (28)$$

So, equation (14) is called the neighborhood version of redefined first Zagreb entropy.

$$\begin{aligned} \mathfrak{G}_{\mathbb{R}ez_{1N}}(\mathfrak{B}) &= \log_2(\mathbb{R}ez_{1N}) - \frac{1}{(\mathbb{R}ez_{1N})} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\frac{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})}{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})} \right] \log_2 \left[\frac{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})}{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})} \right]. \end{aligned} \quad (29)$$

(xv) Neighborhood version of redefined second Zagreb entropy.

If $\mathbb{I}(uv) = \mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v}) / \mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})} \right] = \mathbb{R}ez_{2N}. \quad (30)$$

So, equation (15) is called the neighborhood version of redefined second Zagreb entropy.

$$\begin{aligned} \mathfrak{G}_{\mathbb{R}ez_{2N}}(\mathfrak{B}) &= \log_2(\mathbb{R}ez_{2N}) - \frac{1}{(\mathbb{R}ez_{2N})} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\frac{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})} \right] \log_2 \left[\frac{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})} \right]. \end{aligned} \quad (31)$$

(xvi) Neighborhood version of atom bond connectivity entropy.

If $\mathbb{I}(uv) = \sqrt{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v}) - 2/\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\sqrt{\frac{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v}) - 2}{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}} \right] = ABC_N. \quad (32)$$

So, equation (16) is called the neighborhood version of atom bond connectivity entropy [31].

$$\begin{aligned} \mathfrak{G}_{ABC_N}(\mathfrak{B}) &= \log_2(ABC_N) - \frac{1}{(ABC_N)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\sqrt{\frac{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v}) - 2}{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}} \right] \log_2 \\ &\cdot \left[\sqrt{\frac{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v}) - 2}{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}} \right]. \end{aligned} \quad (33)$$

(xvii) Neighborhood version of geometric arithmetic entropy.

If $\mathbb{I}(uv) = 2 \times \sqrt{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})} / \mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})$, then

$$\sum_{uv \in \mathfrak{G}(\mathfrak{B})} \mathbb{I}(uv) = \sum_{uv \in \mathfrak{G}(\mathfrak{B})} \left[\frac{2 \times \sqrt{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}}{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})} \right] = GA_N. \quad (34)$$

So, equation (17) is called the neighborhood version of geometric arithmetic entropy [31].

$$\begin{aligned} \mathfrak{G}_{GA_N}(\mathfrak{B}) &= \log_2(GA_N) - \frac{1}{(GA_N)} \sum_{i=1}^q \sum_{uv \in \mathfrak{G}_i(\mathfrak{B})} \\ &\cdot \left[\frac{2 \times \sqrt{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}}{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})} \right] \log_2 \\ &\cdot \left[\frac{2 \times \sqrt{\mathfrak{A}(\mathbf{u}) \times \mathfrak{A}(\mathbf{v})}}{\mathfrak{A}(\mathbf{u}) + \mathfrak{A}(\mathbf{v})} \right]. \end{aligned} \quad (35)$$

2. Curvilinear Regression Analysis of Proposed Entropies

In this section, we analyze the entropies given above with the following physical characteristics of the benzene derivatives [32, 33]: critical pressure (\mathcal{CP}), critical temperature (\mathcal{CT}), critical volume (\mathcal{CV}), Gibb's energy (\mathcal{qE}), $\log(P)$, molar refractivity (\mathcal{MR}), and Henry's law (\mathcal{HL}). The experimental values of physical characteristics of benzene derivatives have been referred to from [34] and presented in Table 1. We have presented the values of the proposed indices for the benzene derivatives in Tables 2 and 3. Figures 3 and 4 illustrate the structure of benzene derivatives.

We analyze the topological indices vis a vis the physical characteristics using the following regression models:

$$\mathfrak{P} = \tilde{a} + \tilde{b}\mathfrak{X}, \quad (36)$$

where \mathfrak{P} is the physical property, \mathfrak{X} is the entropy, and \tilde{a} and \tilde{b} represent the coefficient and constant, respectively. For the seven physicochemical properties, we found the correlation between the properties and the seventeen entropies proposed by us. We now present the analysis of the linear model based on the R^2 value. Based on the recommendations of the International Academy of Mathematical Chemistry (IAMC), we have only considered regression models with $R^2 \geq 0.8$.

2.1. Linear Regression Models. Using equation (36), we obtained the linear regression models (LRM) for the seven physicochemical properties via each of the proposed indices, and the results are presented in Tables 4–9.

Table 4 shows the relation between entropy and critical temperature. In Table 4, we can easily see that all the entropies show the highest positive correlation with critical temperature. The most significant regression models are shown as follows:

$$\begin{aligned} \mathcal{CT} &= -159.668 + 185.780\mathfrak{G}_{GA_N} \\ \mathcal{CT} &= -168.156 + 191.581\mathfrak{G}_{\text{NID}_6} \\ \mathcal{CT} &= -111.034 + 177.475\mathfrak{G}_{\text{NID}_4} \\ \mathcal{CT} &= -161.636 + 187.887\mathfrak{G}_{\mathbb{R}ez_{1N}} \\ \mathcal{CT} &= -148.444 + 182.909\mathfrak{G}_{ABC_N} \\ \mathcal{CT} &= -165.387 + 664\mathfrak{G}_{\mathbb{R}ez_{2N}}. \end{aligned} \quad (37)$$

Figure 5 shows that all the points fall near the fitted line. From all entropies, the fifth geometric arithmetic entropy

TABLE 1: The physical characteristics of benzene derivatives.

Chemical structures	CP	HL	GE	CT	$\log(P)$	CV	MR
Benzene (\mathcal{C}_1)	47.69	0.66	121.68	323.79	2.03	263.5	25.28
Naphthalene (\mathcal{C}_2)	38.97	1.67	252.38	484.95	3.03	409.5	42.45
Phenanthrene (\mathcal{C}_3)	32.43	2.68	383.08	586.11	4.03	555.5	59.62
Anthracene (\mathcal{C}_4)	32.43	2.68	383.08	586.11	4.03	555.5	59.62
Chrysene (\mathcal{C}_5)	27.41	3.69	513.78	650.8	5.03	701.5	76.79
Benz[a]anthrene (\mathcal{C}_6)	27.41	3.69	513.78	650.8	5.03	701.5	76.79
Triphenylene (\mathcal{C}_7)	27.41	3.69	513.78	650.8	5.03	701.5	76.79
Tetracene (\mathcal{C}_8)	27.41	3.69	513.78	650.8	5.9	701.5	76.79
Benzo[a]pyrene (\mathcal{C}_9)	26.08	4.48	621.88	689.17	5.34	765.5	85.53
Benzo[e]pyrene (\mathcal{C}_{10})	26.08	4.48	621.88	689.17	5.34	765.5	85.53
Perylene (\mathcal{C}_{11})	26.08	4.48	621.88	689.17	5.34	765.5	85.53
Benzo[ghi]perylene (\mathcal{C}_{12})	24.85	5.27	729.98	728.06	5.66	829.5	94.28
Dibenzo[a, c]anthracene (\mathcal{C}_{13})	23.47	4.7	644.48	714.53	6.02	847.5	93.96
Dibenzo[a, h]anthracene (\mathcal{C}_{14})	23.47	4.7	644.48	714.53	6.02	847.5	93.96
Dibenzo[a, j]anthracene (\mathcal{C}_{15})	23.47	4.7	644.48	714.53	6.02	847.5	93.96
Picene (\mathcal{C}_{16})	23.47	4.7	644.48	714.53	6.02	847.5	93.96
Coronene (\mathcal{C}_{17})	23.7	6.06	838.08	767.68	5.98	893.5	103.02
Pyrene (\mathcal{C}_{18})	30.73	3.47	491.18	625.65	5.08	619.5	68.36

TABLE 2: Numerical values of neighborhood version of entropies.

Compound	\mathcal{E}_{F_N}	\mathcal{E}_{M_N}	\mathcal{E}_{HM_N}	\mathcal{E}_{ND_1}	\mathcal{E}_{ND_2}	\mathcal{E}_{ND_3}	\mathcal{E}_{ND_4}	\mathcal{E}_{ND_5}	\mathcal{E}_{ND_6}
\mathcal{C}_1	2.5850	2.5850	2.5850	2.5849	2.5849	2.5849	2.5849	2.5849	2.5849
\mathcal{C}_2	3.3565	3.3599	3.3583	3.4344	3.4532	3.2416	3.4359	3.4591	3.3767
\mathcal{C}_3	3.8466	3.8645	3.8647	3.9651	3.9911	3.7126	3.9032	3.9991	3.8986
\mathcal{C}_4	3.9062	3.9048	3.9056	3.9739	3.9928	3.8095	3.9710	3.9997	3.8981
\mathcal{C}_5	4.2601	4.2575	4.2591	4.3568	3.3413	4.1134	3.7453	4.3912	4.2926
\mathcal{C}_6	4.2712	4.2832	4.2720	4.3628	4.3842	4.1699	4.3599	4.3918	4.3107
\mathcal{C}_7	4.2158	4.2103	4.2135	4.3429	4.3794	4.0333	4.3426	4.3908	4.3401
\mathcal{C}_8	4.3140	4.3120	4.3131	4.3694	4.3856	4.2373	4.3642	4.3921	4.3302
\mathcal{C}_9	4.4504	4.4433	4.4485	4.3480	4.5756	4.2959	4.5477	4.5843	4.4903
\mathcal{C}_{10}	4.4259	4.3587	4.3633	4.5403	4.2838	4.4725	4.5395	4.5839	4.4729
\mathcal{C}_{11}	4.4286	4.4206	4.4249	4.5410	4.5738	4.2550	4.5408	4.5840	4.4736
\mathcal{C}_{12}	4.6133	4.6055	4.6097	4.7157	4.7451	5.2290	4.7159	4.7542	4.6580
\mathcal{C}_{13}	4.5561	4.5506	4.5538	4.6600	4.6984	4.3997	4.6580	4.6935	4.5958
\mathcal{C}_{14}	4.5925	4.5901	4.5915	4.6704	4.6922	4.4770	4.6671	4.6998	4.6181
\mathcal{C}_{15}	4.5925	4.5901	4.5915	4.6704	4.6922	4.4770	4.6671	4.6998	4.6181
\mathcal{C}_{16}	4.5753	4.5711	4.5736	4.6659	4.6912	4.4366	4.6640	4.6991	4.6118
\mathcal{C}_{17}	4.7805	4.7735	4.7771	4.8729	4.8988	4.6252	4.8752	4.9064	4.8235
\mathcal{C}_{18}	4.1111	4.1079	4.1096	4.2131	4.2396	4.1095	4.2160	4.2476	4.1527

TABLE 3: Numerical values of neighborhood version of entropies.

Compound	\mathcal{E}_{SK_N}	$\mathcal{E}_{SK_{1N}}$	$\mathcal{E}_{SK_{2N}}$	\mathcal{E}_{mR_N}	$\mathcal{E}_{Rez_{1N}}$	$\mathcal{E}_{Rez_{2N}}$	\mathcal{E}_{ABC_N}	\mathcal{E}_{GA_N}
\mathcal{C}_1	2.5849	2.5849	2.5849	2.5849	2.5849	2.5849	2.5849	2.5849
\mathcal{C}_2	3.4338	3.3599	3.3624	3.4244	3.4367	3.4350	3.4561	3.4594
\mathcal{C}_3	3.2830	3.6126	3.8647	3.9533	3.9096	3.9479	3.9950	3.9999
\mathcal{C}_4	3.9265	3.9048	3.9056	3.8641	3.9603	3.9738	3.9959	3.9990
\mathcal{C}_5	4.3567	4.2575	4.1429	4.3448	4.3569	4.3491	3.3869	4.3922
\mathcal{C}_6	4.3628	4.2832	4.2841	4.3182	4.3603	4.3627	4.3875	4.3923
\mathcal{C}_7	4.3431	4.2103	4.2985	4.3334	4.3436	4.3426	3.3847	4.3922
\mathcal{C}_8	4.3695	4.3120	4.3131	4.3609	4.3642	4.3691	3.3884	4.3923
\mathcal{C}_9	4.5488	4.4462	4.4485	4.5563	4.5480	4.5482	4.5791	4.5849
\mathcal{C}_{10}	4.5409	4.4183	4.4224	4.5360	4.5397	4.5395	4.7898	4.5849
\mathcal{C}_{11}	4.5417	4.4206	4.4249	4.2940	4.5213	4.5401	4.5777	4.5849
\mathcal{C}_{12}	4.7165	4.6353	4.6097	4.7149	4.7158	4.7148	4.7483	4.7548
\mathcal{C}_{13}	4.6603	4.5506	4.7847	4.6495	4.6588	4.6208	4.6940	4.7004
\mathcal{C}_{14}	4.6535	4.5901	4.5915	4.6583	4.6675	4.6702	4.6702	4.6955
\mathcal{C}_{15}	4.6535	4.5901	4.5915	4.6583	4.6675	4.6702	4.6702	4.6955
\mathcal{C}_{16}	4.6660	4.5711	4.5736	4.6537	4.6647	4.6656	4.6949	4.7004
\mathcal{C}_{17}	4.8736	4.7735	4.7771	4.8707	4.8750	4.8819	4.9012	4.9069
\mathcal{C}_{18}	4.2132	4.1079	4.1096	4.2111	4.2162	4.2129	4.2426	4.2479

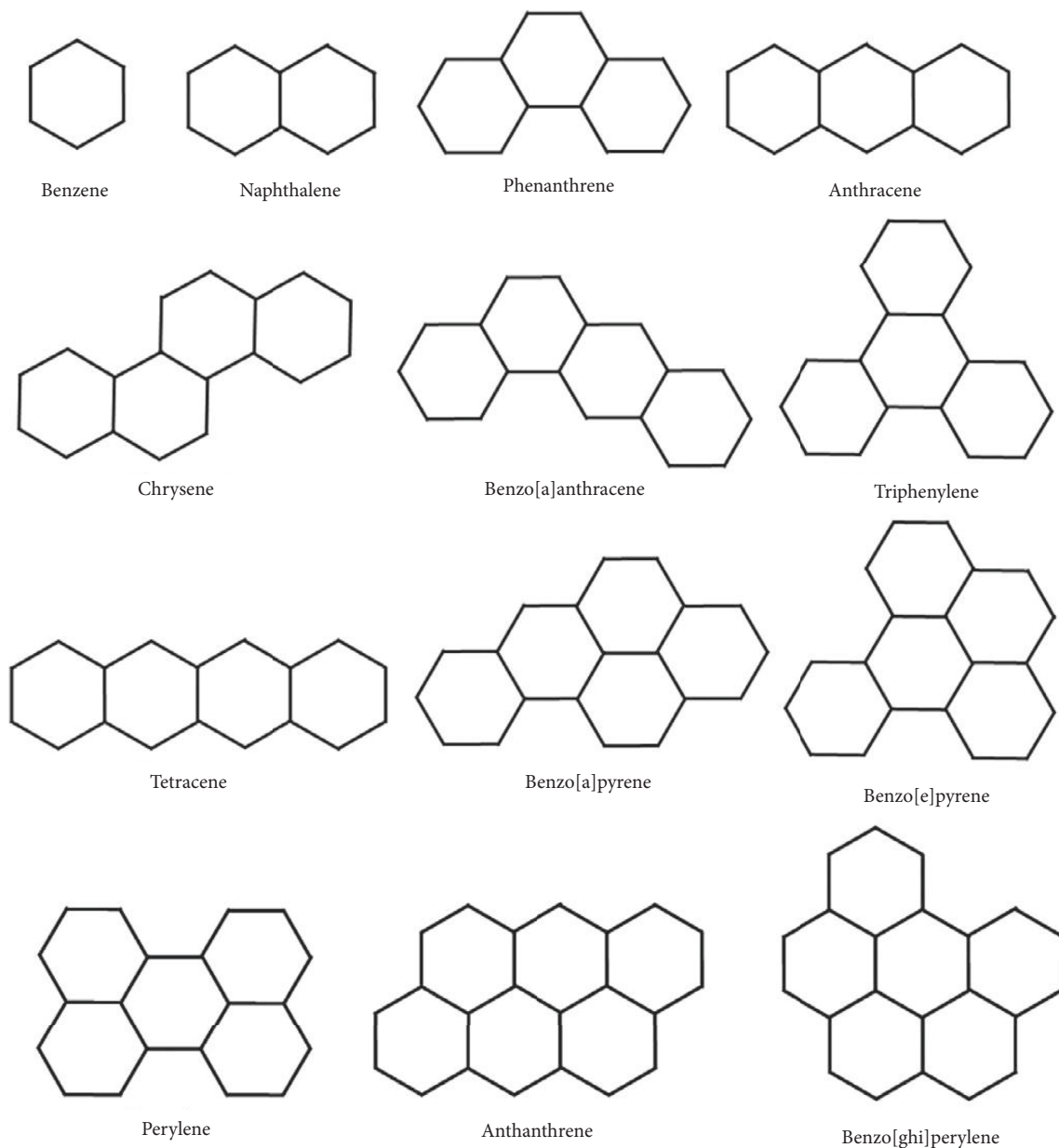


FIGURE 3: An illustration of benzene derivatives for the first type.

shows the best relation with critical temperature (\mathcal{CT}). So, the critical temperature can be predicted by using the fifth geometric arithmetic entropy.

Table 5 shows the relation between entropy and critical pressure (\mathcal{CP}), and all the entropies show the highest positive correlation with critical pressure. The most significant regression models are shown as follows:

$$\begin{aligned}
 \mathcal{CP} &= 77.137 - 11.477\mathcal{G}_{\text{SK}_{2N}} \\
 \mathcal{CP} &= 96.285 - 11.005\mathcal{G}_{\text{ND}_4} \\
 \mathcal{CP} &= 77.014 - 11.192\mathcal{G}_{\text{ND}_5} \\
 \mathcal{CP} &= 77.547 - 11.545\mathcal{G}_{\text{ND}_6} \\
 \mathcal{CP} &= 76.958 - 11.329\mathcal{G}_{\text{mR}_N} \\
 \mathcal{CP} &= 77.121 - 11.314\mathcal{G}_{\text{Rez}_{1N}}.
 \end{aligned}
 \tag{38}$$

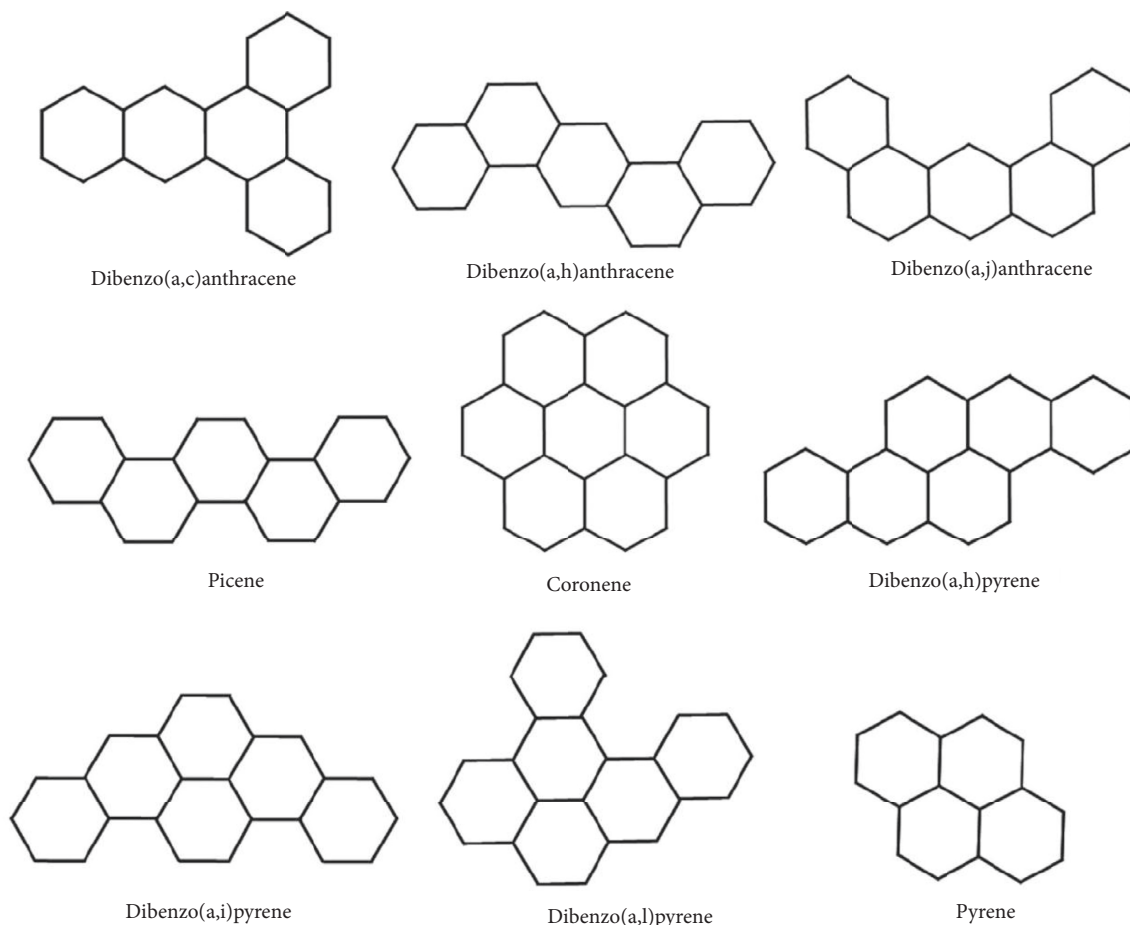


FIGURE 4: An illustration of benzene derivatives for the second type.

TABLE 4: The significant LRM: critical temperature of benzene derivatives on indices.

Entropies	\mathfrak{R}	\mathfrak{R} -square	Adj (\mathfrak{R}^2)	\mathfrak{s}
Modified neighborhood version of forgotten entropy	0.998	0.996	0.996	6.66225
Neighborhood version of second Zagreb entropy	0.998	0.996	0.996	6.87851
First ND entropy	0.998	0.997	0.996	6.59836
Second ND entropy	0.999	0.997	0.997	5.94872
Third ND entropy	0.999	0.997	0.996	6.18795
Fourth ND entropy	0.999	0.998	0.996	6.41912
Fifth ND entropy	0.999	0.998	0.997	6.12268
Sixth ND entropy	0.999	0.998	0.996	6.43054
SK entropy	0.961	0.923	0.918	29.78877
First SK entropy	0.997	0.993	0.992	9.06386
Second SK entropy	0.997	0.994	0.993	8.62473
Neighborhood version of modified Randic entropy	0.997	0.995	0.993	8.55077
Neighborhood version of redefined first Zagreb entropy	0.999	0.998	0.997	5.48691
Fourth atom bond connectivity entropy	0.999	0.998	0.997	5.71456
Neighborhood version of hyper-Zagreb entropy	0.998	0.995	0.995	7.23697
Neighborhood version of redefined second Zagreb entropy	0.999	0.998	0.997	5.4923
Fifth geometric arithmetic entropy	0.999	.998	0.997	5.45456

From all the entropies, the second *SK* entropy shows the best relation with critical pressure (\mathcal{CP}), and all the points fall near the fitted line shown in Figure 6. So, the critical

pressure (\mathcal{CP}) can be predicted by using the second *SK* entropy.

Table 6 shows the relation between entropy and critical volume. From Table 6, we can easily see that all the entropies

TABLE 5: The significant LRM: critical pressure (CP) of benzene derivatives on indices.

Entropies	\mathcal{R}	\mathcal{R} -square	Adj (\mathcal{R}^2)	\mathcal{S}
Neighborhood version of second Zagreb entropy	0.993	0.985	0.983	0.81336
First ND entropy	0.993	0.986	0.983	0.8299
Second ND entropy	0.993	0.986	0.981	0.85676
Third ND entropy	0.994	0.988	0.983	0.812
Fourth ND entropy	0.994	0.988	0.982	0.8429
Fifth ND entropy	0.994	0.989	0.98	0.8797
Sixth ND entropy	0.995	0.989	0.979	0.90475
SK entropy	0.958	0.917	0.912	1.87022
First SK entropy	0.991	0.982	0.98	0.88984
Second SK entropy	0.995	0.989	0.987	0.72501
Neighborhood version of modified Randic entropy	0.995	0.989	0.986	0.72720
Neighborhood version of redefined first Zagreb entropy	0.995	0.989	0.985	0.77312
Fourth atom bond connectivity entropy	0.995	0.990	0.984	0.7966
Neighborhood version of hyper-Zagreb entropy	0.992	0.985	0.984	0.79918
Neighborhood version of redefined second Zagreb entropy	0.992	0.985	0.983	0.825
Fifth geometric arithmetic entropy	0.994	0.988	0.986	0.75756

TABLE 6: The significant LRM: critical volume of benzene derivatives on indices.

Entropies	\mathcal{R}	\mathcal{R} -square	Adj (\mathcal{R}^2)	\mathcal{S}
Modified neighborhood version of forgotten entropy	0.981	0.963	0.961	33.08152
Neighborhood version of second Zagreb entropy	0.982	0.964	0.959	33.90248
First ND entropy	0.982	0.965	0.957	34.7795
Second ND entropy	0.982	0.965	0.954	36.03779
Third ND entropy	0.982	0.965	0.95	37.50893
Fourth ND entropy	0.982	0.965	0.946	39.09405
Fifth ND entropy	0.991	0.983	0.967	30.46046
Sixth ND entropy	0.987	0.974	0.956	35.1254
SK entropy	0.961	0.923	0.918	47.88923
First SK entropy	0.982	0.965	0.961	33.26689
Second SK entropy	0.984	0.968	0.961	33.15523
Neighborhood version of modified Randic entropy	0.984	0.968	0.958	34.26668
Neighborhood version of redefined first Zagreb entropy	0.985	0.971	0.959	34.09436
Fourth atom bond connectivity entropy	0.986	0.971	0.956	35.26197
Neighborhood version of hyper-Zagreb entropy	0.981	0.962	0.959	33.85292
Neighborhood version of redefined second Zagreb entropy	0.982	0.964	0.959	33.95369
Fifth geometric arithmetic entropy	0.982	0.964	0.956	35.14404

TABLE 7: The significant LRM: Gibb's energy (GE) of benzene derivatives on indices.

Entropies	\mathcal{R}	\mathcal{R} -square	Adj (\mathcal{R}^2)	\mathcal{S}
Modified neighborhood version of forgotten entropy	0.957	0.917	0.911	51.08458
Neighborhood version of second Zagreb entropy	0.960	0.922	0.912	50.92216
First ND entropy	0.962	0.925	0.908	51.96242
Second ND entropy	0.963	0.927	0.904	53.0685
Third ND entropy	0.967	0.935	0.909	51.91691
Fourth ND entropy	0.967	0.936	0.901	54.00602
Fifth ND entropy	0.973	0.946	0.908	52.04307
Sixth ND entropy	0.978	0.956	0.917	49.48688
SK entropy	0.943	0.889	0.882	58.99765
First SK entropy	0.959	0.92	0.91	51.58078
Second SK entropy	0.960	0.921	0.904	53.17509
Neighborhood version of modified Randic entropy	0.960	0.922	0.898	54.93049
Neighborhood version of redefined first Zagreb entropy	0.960	0.922	0.889	57.16546
Fourth atom bond connectivity entropy	0.960	0.922	0.879	59.6619
Neighborhood version of hyper-Zagreb entropy	0.955	0.913	0.907	52.24284
Neighborhood version of redefined second Zagreb entropy	0.956	0.913	0.902	53.85496
Fifth geometric arithmetic entropy	0.959	0.92	0.903	53.56609

TABLE 8: The significant LRM: $\log(P)$ of benzene derivatives on indices.

Entropies	\mathfrak{R}	\mathfrak{R} -square	Adj (\mathfrak{R}^2)	\mathfrak{s}
Modified neighborhood version of forgotten entropy	0.969	0.94	0.936	0.28258
Neighborhood version of second Zagreb entropy	0.970	0.94	0.932	0.29159
First ND entropy	0.970	0.94	0.928	0.30098
Second ND entropy	0.971	0.943	0.926	0.30508
Third ND entropy	0.971	0.943	0.92	0.31671
Fourth ND entropy	0.972	0.944	0.914	0.32831
Fifth ND entropy	0.981	0.963	0.936	0.28207
Sixth ND entropy	0.985	0.971	0.945	0.26278
SK entropy	0.951	0.905	0.899	0.35614
First SK entropy	0.971	0.943	0.935	0.28406
Second SK entropy	0.972	0.945	0.933	0.28894
Neighborhood version of modified Randic entropy	0.972	0.945	0.928	0.29977
Neighborhood version of redefined first Zagreb entropy	0.977	0.955	0.936	0.28365
Fourth atom bond connectivity entropy	0.977	0.955	0.93	0.29626
Neighborhood version of hyper-Zagreb entropy	0.969	0.94	0.936	0.2827
Neighborhood version of redefined second Zagreb entropy	0.975	0.951	0.944	0.2637
Fifth geometric arithmetic entropy	0.975	0.951	0.94	0.27288

TABLE 9: The significant LRM: molar refractivity (MR) of benzene derivatives on indices.

Entropies	\mathfrak{R}	\mathfrak{R} -square	Adj (\mathfrak{R}^2)	\mathfrak{s}
Modified neighborhood version of forgotten entropy	0.981	0.962	0.96	4.02512
Neighborhood version of second Zagreb entropy	0.982	0.964	0.959	4.09119
First ND entropy	0.982	0.964	0.957	4.1829
Second ND entropy	0.982	0.964	0.954	4.34063
Third ND entropy	0.982	0.965	0.95	4.49344
Fourth ND entropy	0.982	0.965	0.946	4.67932
Fifth ND entropy	0.987	0.975	0.957	4.18104
Sixth ND entropy	0.992	0.983	0.969	3.56484
SK entropy	0.961	0.924	0.92	5.70614
First SK entropy	0.982	0.965	0.96	4.03334
Second SK entropy	0.983	0.966	0.958	4.10153
Neighborhood version of modified Randic entropy	0.983	0.966	0.955	4.25288
Neighborhood version of redefined first Zagreb entropy	0.984	0.968	0.954	4.31552
Fourth atom bond connectivity entropy	0.984	0.968	0.951	4.47577
Neighborhood version of hyper-Zagreb entropy	0.980	0.96	0.958	4.14024
Neighborhood version of redefined second Zagreb entropy	0.980	0.961	0.956	4.21432
Fifth geometric arithmetic entropy	0.981	0.962	0.953	4.34898

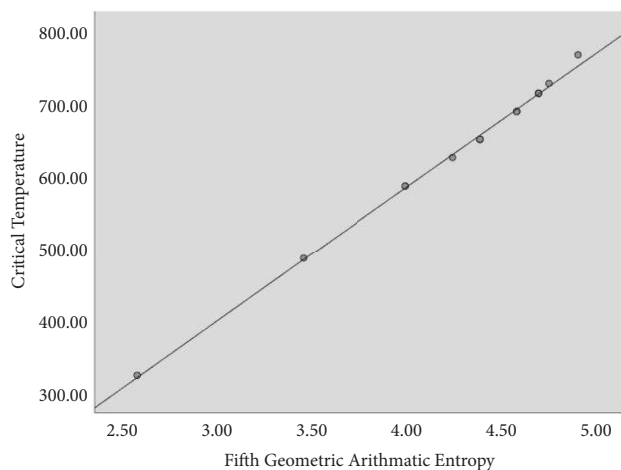


FIGURE 5: Graphical representation of LRM between critical temperature and the fifth geometric arithmetic entropy.

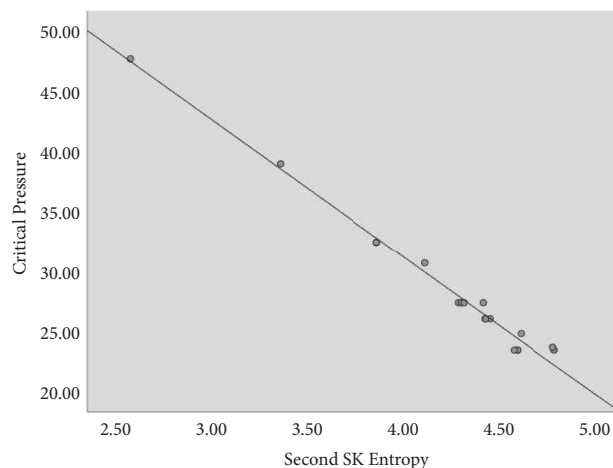


FIGURE 6: Graphical representation of LRM between critical pressure (CP) and the second SK entropy.

show the highest positive correlation with critical volume. The most significant regression models are shown as follows:

$$\begin{aligned}
 \mathcal{CV} &= -569.955 + 293.079\mathfrak{E}_{\text{ND}_5} \\
 \mathcal{CV} &= -589.308 + 303.572\mathfrak{E}_{\text{ND}_6} \\
 \mathcal{CV} &= -576.671 + 297.184\mathfrak{E}_{\text{Rez}_{1N}} \\
 \mathcal{CV} &= -551.360 + 288.287\mathfrak{E}_{\text{ABC}_N} \\
 \mathcal{CV} &= -577.343 + 65.676\mathfrak{E}_{\text{SK}_{2N}} \\
 \mathcal{CV} &= -573.522 + 297.843\mathfrak{E}_{\text{mR}_N}.
 \end{aligned}
 \tag{39}$$

From all the entropies, the fifth *ND* entropy shows the best relation with critical volume (\mathcal{CV}), and all the points fall near the fitted line as can be seen in Figure 7. So, the critical temperature can be predicted by using the fifth *ND* entropy.

Table 7 shows the relation between entropy and Gibb's energy ($q\mathcal{E}$) of benzene derivatives. From Table 7, we can easily see that all the entropies show the highest positive correlation with Gibb's energy ($q\mathcal{E}$).

$$\begin{aligned}
 q\mathcal{E} &= -751.66 + 303.591\mathfrak{E}_{\text{ND}_6} \\
 q\mathcal{E} &= -732.155 + 293.063\mathfrak{E}_{\text{ND}_5} \\
 q\mathcal{E} &= -674.923 + 284.469\mathfrak{E}_{\text{ND}_4} \\
 q\mathcal{E} &= -639.259 + 283.942\mathfrak{E}_{\text{ND}_3} \\
 q\mathcal{E} &= -725.293 + 293.202\mathfrak{E}_{\text{SK}_{2N}} \\
 q\mathcal{E} &= -739.593 + 297.729\mathfrak{E}_{\text{ND}_1}.
 \end{aligned}
 \tag{40}$$

Of all the entropies, the fifth *ND* entropy shows the best relation with Gibb's energy ($q\mathcal{E}$), and all the points fall near the fitted line as seen in Figure 8. So, Gibb's energy can be predicted by using the sixth *ND* entropy.

Table 8 shows the relation between entropy and $\log(P)$. From Table 8, we can easily see that all the entropies show the highest positive correlation with critical volume. The most significant regression models are shown as follows:

$$\begin{aligned}
 \log(P) &= -3.443 + 1.998\mathfrak{E}_{\text{ND}_6} \\
 \log(P) &= -3.304 + 1.927\mathfrak{E}_{\text{ND}_5} \\
 \log(P) &= -3.159 + 1.890\mathfrak{E}_{\text{ND}_4} \\
 \log(P) &= -3.357 + 1.956\mathfrak{E}_{\text{Rez}_{1N}} \\
 \log(P) &= -3.300 + 1.925\mathfrak{E}_{\text{GA}_N} \\
 \log(P) &= -3.371 + 1.958\mathfrak{E}_{\text{Rez}_{2N}}.
 \end{aligned}
 \tag{41}$$

From all the entropies, the sixth *ND* entropy shows the best relation with $\log(P)$, and all the points fall near the fitted line as can be seen in Figure 9. So, the $\log(P)$ can be predicted by using the sixth *ND* entropy.

Table 9 shows the relation between entropy and molar refractivity (\mathcal{MR}) of benzene derivatives. From Table 9, we can easily see that all the entropies show the highest positive correlation with molar refractivity (\mathcal{MR}).

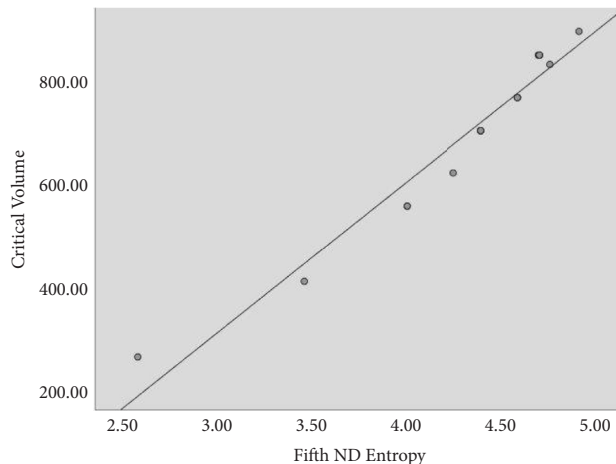


FIGURE 7: Graphical representation of LRM between critical volume and the fifth *ND* entropy.

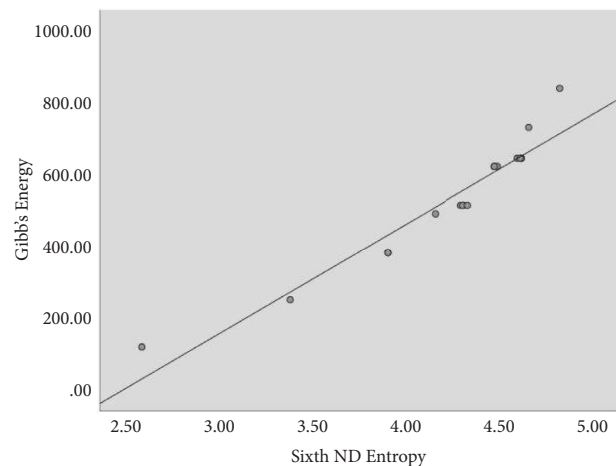


FIGURE 8: Graphical representation of LRM between Gibb's energy (GE) and the sixth *ND* entropy.

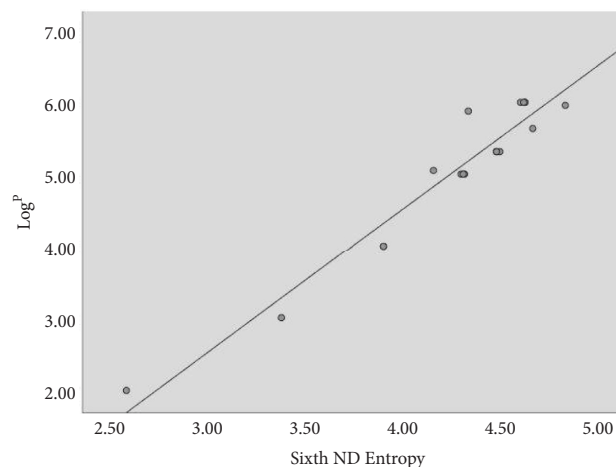


FIGURE 9: Graphical representation of LRM between $\log(P)$ and the sixth *ND* entropy.

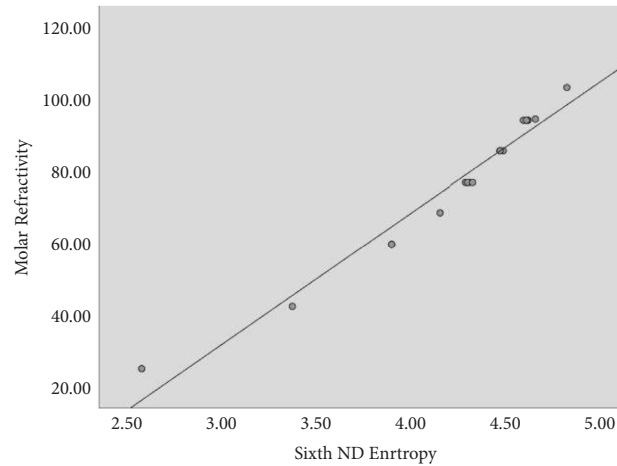


FIGURE 10: Graphical representation of LRM between molar refractivity and the sixth ND entropy.

TABLE 10: The significant LRM: Henry's law of benzene derivatives on indices.

Entropies	\mathfrak{R}	\mathfrak{R} -square	Adj (\mathfrak{R}^2)	\mathfrak{s}
Modified neighborhood version of forgotten entropy	0.962	0.926	0.921	0.36535
Neighborhood version of second Zagreb entropy	0.965	0.931	0.922	0.36445
First ND entropy	0.966	0.933	0.919	0.37174
Second ND entropy	0.967	0.935	0.915	0.38046
Third ND entropy	0.970	0.942	0.918	0.37439
Fourth ND entropy	0.971	0.942	0.911	0.38944
Fifth ND entropy	0.976	0.952	0.919	0.37152
Sixth ND entropy	0.981	0.962	0.929	0.3485
SK entropy	0.947	0.897	0.89	0.43156
First SK entropy	0.964	0.93	0.92	0.36835
Second SK entropy	0.964	0.93	0.915	0.38044
Neighborhood version of modified Randic entropy	0.965	0.93	0.909	0.39337
Neighborhood version of redefined first Zagreb entropy	0.965	0.93	0.901	0.40943
Fourth atom bond connectivity entropy	0.965	0.931	0.893	0.42717
Neighborhood version of hyper-Zagreb entropy	0.960	0.922	0.918	0.37422
Neighborhood version of redefined second Zagreb entropy	0.961	0.923	0.912	0.38616
Fifth geometric arithmetic entropy	0.963	0.928	0.913	0.38561

$$\begin{aligned}
 MR &= -77.645 + 36.463\mathfrak{C}_{\text{ND}_6} \\
 MR &= -75.316 + 35.202\mathfrak{C}_{\text{ND}_5} \\
 MR &= -76.136 + 35.698\mathfrak{C}_{\text{Rez}_{1N}} \\
 MR &= -73.151 + 34.642\mathfrak{C}_{\text{ABC}_N} \\
 MR &= -75.860 + 36.134\mathfrak{C}_{\text{SK}_{2N}} \\
 MR &= -75.730 + 35.771\mathfrak{C}_{\text{intR}_N}
 \end{aligned}
 \tag{42}$$

Of all the entropies, the sixth ND entropy shows the best relation with molar refractivity (MR), and all the points fall near the fitted line as seen in Figure 10. So, the molar refractivity can be predicted by using the sixth ND entropy.

Table 10 shows the relation between entropy and Henry's law. From Table 10, we can easily see that all the entropies show the highest positive correlation with Henry's law. The most significant regression models are shown as follows:

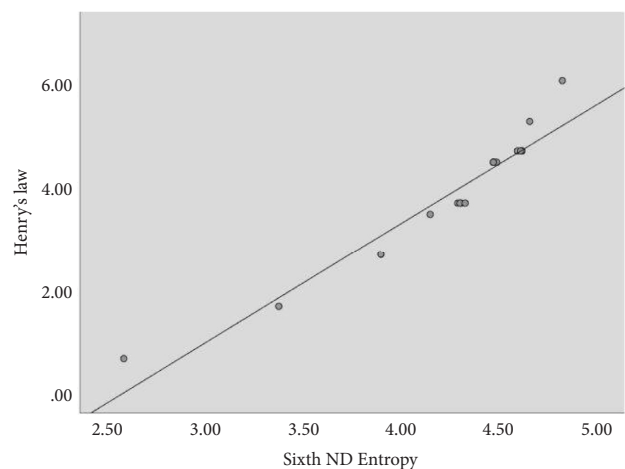


FIGURE 11: Graphical representation of LRM between Henry's law and the sixth ND entropy.

$$\begin{aligned}
 \mathcal{H}L &= -5.991 + 2.318\mathbb{G}_{\text{ND}_6}, \\
 \mathcal{H}L &= -5.842 + 2.237\mathbb{G}_{\text{ND}_5}, \\
 \mathcal{H}L &= -5.395 + 2.169\mathbb{G}_{\text{ND}_4}, \\
 \mathcal{H}L &= -5.102 + 2.160\mathbb{G}_{\text{ND}_3}, \\
 \mathcal{H}L &= -5.793 + 2.239\mathbb{G}_{\text{ND}_2}, \\
 \mathcal{H}L &= -5.902 + 2.074\mathbb{G}_{\text{ND}_1}.
 \end{aligned}
 \tag{43}$$

From all the entropies, the sixth ND entropy shows the best relation with Henry's law ($\mathcal{H}L$), and all the points fall near the fitted line as can be seen in Figure 11. So, Henry's law ($\mathcal{H}L$) can be predicted by using the sixth ND entropy.

3. Concluding Remarks

Quantitative structure-property relationships (QSPRs) mathematically link physical or chemical properties with the structure of a molecule. Entropies are defined on molecular structures for a better understanding of the physical features [35] and chemical reactivity. In this paper, we developed the QSPR between ND entropy and the physical characteristics of benzene derivatives. Based on the linear regression model, we analyzed that critical temperature ($\mathcal{C}T$), critical pressure ($\mathcal{C}P$), and critical volume ($\mathcal{C}V$) can be predicted through the fifth geometric arithmetic entropy, second SK entropy, and fifth ND entropy, respectively. Other remaining physical characteristics such as Gibb's energy ($q\mathcal{E}$), $\log(P)$, molar refractivity ($\mathcal{M}R$), and Henry's law ($\mathcal{H}L$) can be predicted by using the sixth ND entropy.

Data Availability

The data used to support the findings of this study are cited at relevant places within the text as references.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Authors' Contributions

This work was equally contributed by all writers.

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