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ARTICLE

Degree-Based Entropy Descriptors of Graphenylene Using Topological Indices

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ABSTRACT

Graph theory plays a significant role in the applications of chemistry, pharmacy, communication, maps, and aeronautical fields. The molecules of chemical compounds are modelled as a graph to study the properties of the compounds. The geometric structure of the compound relates to a few physical properties such as boiling point, enthalpy, π-electron energy, and molecular weight. The article aims to determine the practical application of graph theory by solving one of the interdisciplinary problems describing the structures of benzenoid hydrocarbons and graphenylene. The topological index is an invariant of a molecular graph associated with the chemical structure, which shows the correlation of chemical structures using many physical, chemical properties and biological activities. This study aims to introduce some novel degree-based entropy descriptors such as ENT_{SO}, ENT_{GH}, ENT_{HG}, ENT_{SS}, ENT_{NSO}, ENT_{NReZ_1}, ENT_{NReZ_2} and ENT_{NSS} using the respective topological indices. Also, the above-mentioned entropy measures and physico-chemical properties of benzenoid hydrocarbons are fitted using linear regression models and calculated for graphenylene structure.

KEYWORDS

Topological descriptors; weighted entropy; graphenylene

1 Introduction

Mathematics and computer science are often used in the applications of research development. One example of such applications is cheminformatics which is a relatively recent area of research in mathematics. The study includes the problem of analysing the structure of a molecule which can be retrieved from the cheminformatics dataset. There are many compounds available in organic and inorganic chemistry whose properties and structures seem promising to search and evaluate the

uses of a substance. The study of the structure of a molecule gives information about its chemical properties [1,2].

Graph theory has been a very useful branch of science, especially in the applications of chemistry. It has a very powerful tool known as the topological index which provides a lot of information about a chemical compound. These topological indices are classified based on degree, distance, and eccentricity [3–6].

Most of these indices have a good correlation with the properties of isomers and benzenoid hydrocarbons, such that the compounds are used for various purposes based on their correlation coefficient [7–9].

Graph theory facilitates the mathematical model of a compound to draw information about the chemical compound. In modelling a compound into a graph, the hydrogen atoms are neglected without losing information about the molecule, as carbon atoms have four chemical bonds whereas hydrogen atom has one chemical bond [10–13].

The recent trends in research have attracted a lot of studies involving information science. It provides a good correlation between the biological and structural properties of compounds. Many scientists have done remarkable findings which led to wide applications in graph theory [14–16].

Graph theory being an ideal tool in the hands of the chemist involves representation, synthesis of compounds and numerous chemical activities. Also, chemists are always interested in breaking and making chemical bonds, resulting in different types of structures [17,18].

The degree of amount of energy dispersed and the measure of unavailability of heat energy for work is termed as the entropy. Originally, Shannon introduced the concept of entropy as a part of the communication theory [19]. According to him, data is communicated as a system consisting of three elements: source, channel and receiver. During his learning, Shannon used various methods to encode, transmit and compress the messages which proved that the entropy denotes an absolute limit on how well data can be compressed from the source to reach the receiver in his famous coding theorem.

The measure of uncertainty refers to the entropy of a probability distribution. Indeed, the result of an analysis conducted can be assumed by taking the numerical value equal to the amount of uncertainty of the outcome of the analysis. Furthermore, studies on graphs and networks were studied by various researchers during the late 1950s. More work on entropy measures was carried out using graph invariants which proved advantageous to study important properties of graphs [20–23].

Several theoretic measures and tools have been developed to study the complexity of the structure of chemical compounds and complex networks. The word entropy is dealt with various ways by researchers involving a variety of problems in different fields like discrete mathematics, biology, chemistry, statistics, etc., in investigating entropies of relational structures. In mathematical chemistry, graph entropy is used to characterize the structure of a graph [24–26].

A class of chemical compounds having at least one benzene ring is termed as a benzenoid. They have a high chemical stability because of its bonding with certain molecules. Benzenoids are aromatic hydrocarbons having significant applications in gasoline additives, dry cleaning, manufacture of synthetic fibres, plastics and products in rubber-like materials [27]. Their applications are growing rapidly in the fields of industrial chemistry particularly, in the products of polymers. The work is carried out for twenty-two benzenoid hydrocarbons refer Fig. 1.

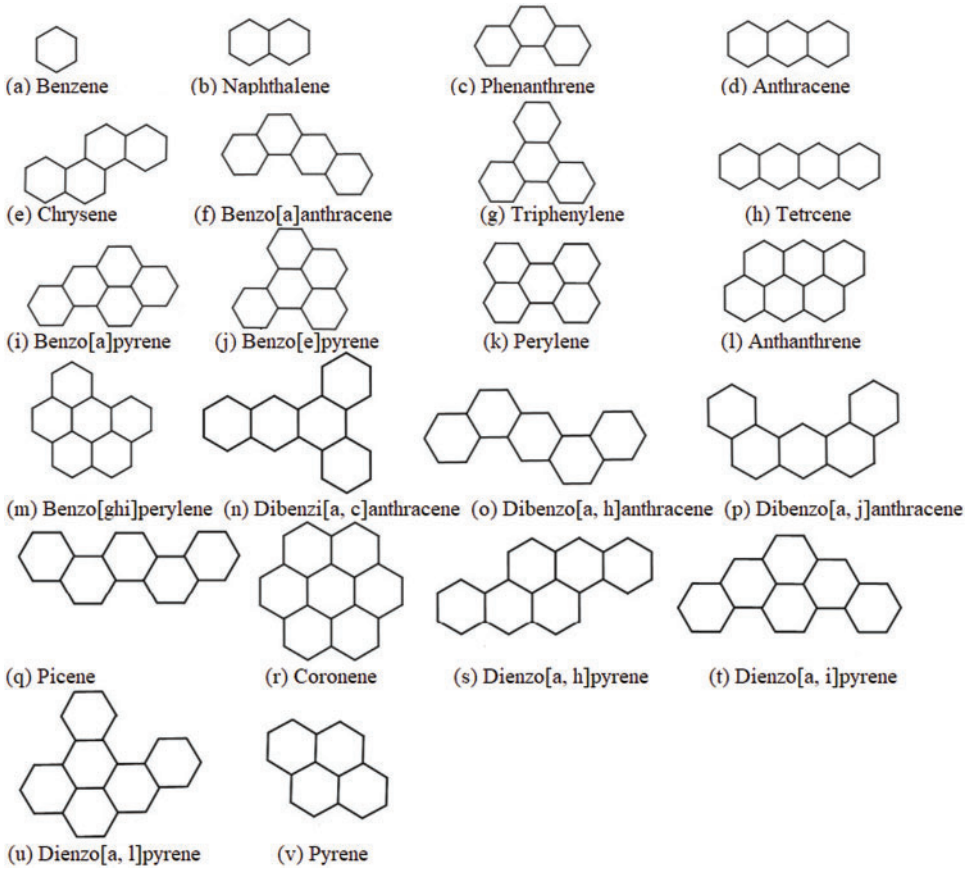


Figure 1: Molecular structure of benzenoid hydrocarbons

Graphenylene is a cyclic hydrocarbon in which each hexagon has a square adjacent to it. Two such hexagons separated by a square are termed as biphenylenes. Chemically, it is a cyclobutadiene ring in between two benzene rings. Biphenylene is a building block of graphenylene which is pale yellowish powder having melting temperature of 110°C. Biphenylene is a hydrocarbon whose chemical formula is $C_{12}H_8$. A 2D graphene is a prospective compound that has significant applications in the next-generation electronic and optical devices. Biphenylene becomes an interesting forerunner of a 2D porous graphene-like molecular network called Graphenylene. This new material has a good dispersion and gap separation in the characterization of delocalized band [28,29].

Numerous studies on graphene have grabbed researchers across the globe due to its magnificent properties and promising potential applications because of its unique 2D structure. Graphene can be wrapped up into fullerenes, carbon nanotubes and even along a specific direction that forms graphene nanoribbon. These have extremely enriched the family of carbon nanomaterials. Also, these studies have created an interest in exploiting new 2D carbon allotropes through both experimental techniques and theoretical calculations [30]. Biphenylene carbon is a product of cyclotrimerization of graphene whose structure is 2D network of hydrogen free carbon atoms.

The main aims/objectives of this work are

- To introduce novel entropy measures.

- To understand their physical/chemical applicability of benzenoid hydrocarbons by regression models.
- To calculate defined entropies of graphenylene structure.

In this article, all standard graph terminologies and notations are referred from [31–33]. In the literature, various studies are carried out using topological indices of which the below mentioned indices are considered in this work.

Definition 1.1. Gutman defined Sombor index [34] as

$$SO(G) = \sum_{\vartheta\omega \in E(G)} \sqrt{(\mathrm{d}(\vartheta))^2 + (\mathrm{d}(\omega))^2}$$

Definition 1.2. Usha et al. [35] defined Geometric-Harmonic index as

$$GH(G) = \sum_{\vartheta\omega \in E(G)} \frac{((\mathrm{d}(\vartheta) + \mathrm{d}(\omega))\left(\sqrt{\mathrm{d}(\vartheta) \times \mathrm{d}(\omega)}\right)}{2}$$

Definition 1.3. Shanmukha et al. [36] defined Harmonic-Geometric index as

$$HG(G) = \sum_{\vartheta\omega \in E(G)} \frac{2}{(\mathrm{d}(\vartheta) + \mathrm{d}(\omega))\left(\sqrt{\mathrm{d}(\vartheta) \times \mathrm{d}(\omega)}\right)}$$

Definition 1.4. Zhao et al. [37] defined SS index as

$$SS(G) = \sum_{\vartheta\omega \in E(G)} \sqrt{\frac{\mathrm{d}(\vartheta) \times \mathrm{d}(\omega)}{\mathrm{d}(\vartheta) + \mathrm{d}(\omega)}}$$

In continuation to SS index, the neighborhood version of SS index is defined as

$$NSS(G) = \sum_{\vartheta\omega \in E(G)} \sqrt{\frac{\mathrm{S}(\vartheta) \times \mathrm{S}(\omega)}{\mathrm{S}(\vartheta) + \mathrm{S}(\omega)}}$$

Definition 1.5. Kulli [38] defined neighborhood Sombor index as

$$NSO(G) = \sum_{\vartheta\omega \in E(G)} \sqrt{(\mathrm{S}(\vartheta))^2 + (\mathrm{S}(\omega))^2}$$

Definition 1.6. Shanmukha et al. [39] defined neighborhood redefined first and second Zagreb indices as

$$NReZ_1(G) = \sum_{\vartheta\omega \in E(G)} \frac{\mathrm{S}(\vartheta) + \mathrm{S}(\omega)}{\mathrm{S}(\vartheta) \times \mathrm{S}(\omega)}$$

$$NReZ_2(G) = \sum_{\vartheta\omega \in E(G)} \frac{\mathrm{S}(\vartheta) \times \mathrm{S}(\omega)}{\mathrm{S}(\vartheta) + \mathrm{S}(\omega)}$$

1.1 Graph Entropy Based on Degree and Edge Weight

The theory of edge weighted graph based on entropy was first introduced by Chen et al. [40] in the year 2014. Let G be an edge weighted graph, denoted by $(V(G), E(G), \psi(\vartheta\omega))$. Here, $V(G)$ and $E(G)$

are the usual notations of the set of vertices and edges respectively, where $\psi(\vartheta\omega)$ denotes the edge weight of the graph G. The edge weight of $\psi(\vartheta\omega)$ is computed by adding the degrees of the vertices ϑ and ω of the edge $\vartheta\omega$. Then, the graph entropy based on edge weight is defined in Eq. (1).

$$ENT_{\psi}(G) = -\sum_{\vartheta'\omega'\in E(G)} \frac{\psi(\vartheta'\omega')}{\sum_{\vartheta\omega\in E(G)}\psi(\vartheta\omega)} log\left[\frac{\psi(\vartheta'\omega')}{\sum_{\vartheta\omega\in E(G)}\psi(\vartheta\omega)}\right] \tag{1}$$

- **Sombor Entropy**

  If $\psi(\vartheta\omega) = \sqrt{\mathrm{d}(\vartheta)^2 + \mathrm{d}(\omega)^2}$, then

  $$\sum_{\vartheta\omega\in E(G)} \psi(\vartheta\omega) = \sum_{\vartheta\omega\in E(G)} \sqrt{\mathrm{d}(\vartheta)^2 + \mathrm{d}(\omega)^2} = SO(G)$$

  Using the definition of Eq. (1) for Sombor index results in Sombor entropy given by

  $$ENT_{SO(G)} = log(SO(G)) - \frac{1}{SO(G)} log\left[\prod_{\vartheta\omega\in E(G)}\left[\sqrt{\mathrm{d}(\vartheta)^2 + \mathrm{d}(\omega)^2}\right]^{\left[\sqrt{\mathrm{d}(\vartheta)^2+\mathrm{d}(\omega)^2}\right]}\right] \tag{2}$$

- **Geometric-Harmonic Entropy**

  If $\psi(\vartheta\omega) = \dfrac{(\mathrm{d}(\vartheta) + \mathrm{d}(\omega))\left(\sqrt{\mathrm{d}(\vartheta)\times\mathrm{d}(\omega)}\right)}{2}$, then

  $$\sum_{\vartheta\omega\in E(G)} \psi(\vartheta\omega) = \sum_{\vartheta\omega\in E(G)} \frac{(\mathrm{d}(\vartheta) + \mathrm{d}(\omega))\left(\sqrt{\mathrm{d}(\vartheta)\times\mathrm{d}(\omega)}\right)}{2} = GH(G)$$

  Using the definition of Eq. (1) for Geometric-Harmonic index results in Geometric-Harmonic entropy given by

  $$ENT_{GH(G)} = log(GH(G))$$
  $$- \frac{1}{GH(G)} log\left[\prod_{\vartheta\omega\in E(G)}\left[\frac{(\mathrm{d}(\vartheta) + \mathrm{d}(\omega))\left(\sqrt{\mathrm{d}(\vartheta)\times\mathrm{d}(\omega)}\right)}{2}\right]^{\left[\frac{(\mathrm{d}(\vartheta) + \mathrm{d}(\omega))\left(\sqrt{\mathrm{d}(\vartheta)\times\mathrm{d}(\omega)}\right)}{2}\right]}\right] \tag{3}$$

- **Harmonic-Geometric Entropy**

  If $\psi(\vartheta\omega) = \dfrac{2}{(\mathrm{d}(\vartheta) + \mathrm{d}(\omega))(\sqrt{\mathrm{d}(\vartheta)\times\mathrm{d}(\omega)})}$, then

  $$\sum_{\vartheta\omega\in E(G)} \psi(\vartheta\omega) = \sum_{\vartheta\omega\in E(G)} \frac{2}{(\mathrm{d}(\vartheta) + \mathrm{d}(\omega))\left(\sqrt{\mathrm{d}(\vartheta)\times\mathrm{d}(\omega)}\right)} = HG(G)$$

  Using the definition of Eq. (1) for Harmonic-Geometric index results in Harmonic-Geometric entropy given by

$$ENT_{HG(G)} = log(HG(G))$$
$$- \frac{1}{HG(G)} log \left[\prod_{\vartheta\omega \in E(G)} \left[\frac{2}{(\mathrm{d}(\vartheta) + \mathrm{d}(\omega)) \left(\sqrt{\mathrm{d}(\vartheta) \times \mathrm{d}(\omega)} \right)} \right]^{\left[\frac{2}{(\mathrm{d}(\vartheta) + \mathrm{d}(\omega)) \left(\sqrt{\mathrm{d}(\vartheta) \times \mathrm{d}(\omega)} \right)} \right]} \right] \tag{4}$$

- **The *SS* Entropy**

If $\psi(\vartheta\omega) = \sqrt{\frac{\mathrm{d}(\vartheta) \times \mathrm{d}(\omega)}{\mathrm{d}(\vartheta) + \mathrm{d}(\omega)}}$, then

$$\sum_{\vartheta\omega \in E(G)} \psi(\vartheta\omega) = \sum_{\vartheta\omega \in E(G)} \sqrt{\frac{\mathrm{d}(\vartheta) \times \mathrm{d}(\omega)}{\mathrm{d}(\vartheta) + \mathrm{d}(\omega)}} = SS(G)$$

Using the definition of Eq. (1) for *SS* index results in *SS* entropy given by

$$ENT_{SS(G)} = log(SS(G)) - \frac{1}{SS(G)} log \left[\prod_{\vartheta\omega \in E(G)} \left[\sqrt{\frac{\mathrm{d}(\vartheta) \times \mathrm{d}(\omega)}{\mathrm{d}(\vartheta) + \mathrm{d}(\omega)}} \right]^{\left[\sqrt{\frac{\mathrm{d}(\vartheta) \times \mathrm{d}(\omega)}{\mathrm{d}(\vartheta) + \mathrm{d}(\omega)}} \right]} \right] \tag{5}$$

- **The Neighborhood Sombor Entropy**

If $\psi(\vartheta\omega) = \sqrt{\mathrm{S}(\vartheta)^2 + \mathrm{S}(\omega)^2}$, then

$$\sum_{\vartheta\omega \in E(G)} \psi(\vartheta\omega) = \sum_{\vartheta\omega \in E(G)} \sqrt{\mathrm{S}(\vartheta)^2 + \mathrm{S}(\omega)^2} = NSO(G)$$

Using the definition of Eq. (1) for neighborhood Sombor index results in neighborhood Sombor entropy given by

$$ENT_{NSO(G)} = log(NSO(G)) - \frac{1}{NSO(G)} log \left[\prod_{\vartheta\omega \in E(G)} \left[\sqrt{\mathrm{S}(\vartheta)^2 + \mathrm{S}(\omega)^2} \right]^{\left[\sqrt{\mathrm{S}(\vartheta)^2 + \mathrm{S}(\omega)^2} \right]} \right] \tag{6}$$

- **The $NReZ_1$ Entropy**

If $\psi(\vartheta\omega) = \frac{\mathrm{S}(\vartheta) + \mathrm{S}(\omega)}{\mathrm{S}(\vartheta) \times \mathrm{S}(\omega)}$, then

$$\sum_{\vartheta\omega \in E(G)} \psi(\vartheta\omega) = \sum_{\vartheta\omega \in E(G)} \frac{\mathrm{S}(\vartheta) + \mathrm{S}(\omega)}{\mathrm{S}(\vartheta) \times \mathrm{S}(\omega)} = NReZ_1(G)$$

Using the definition of Eq. (1) for $NReZ_1$ index results in $NReZ_1$ entropy given by

$$ENT_{NReZ_1(G)} = log(NReZ_1(G)) - \frac{1}{NReZ_1(G)} log\left[\prod_{\vartheta\omega\in E(G)}\left[\frac{S(\vartheta)+S(\omega)}{S(\vartheta)\times S(\omega)}\right]^{\left[\frac{S(\vartheta)+S(\omega)}{S(\vartheta)\times S(\omega)}\right]}\right] \tag{7}$$

- **The $NReZ_2$ Entropy**

  If $\psi(\vartheta\omega) = \frac{S(\vartheta)\times S(\omega)}{S(\vartheta)+S(\omega)}$, then

  $$\sum_{\vartheta\omega\in E(G)} \psi(\vartheta\omega) = \sum_{\vartheta\omega\in E(G)} \frac{S(\vartheta)\times S(\omega)}{S(\vartheta)+S(\omega)} = NReZ_2(G)$$

  Using the definition of Eq. (1) for $NReZ_2$ index results in $NReZ_2$ entropy given by

$$ENT_{NReZ_2(G)} = log(NReZ_2(G)) - \frac{1}{NReZ_2(G)} log\left[\prod_{\vartheta\omega\in E(G)}\left[\frac{S(\vartheta)\times S(\omega)}{S(\vartheta)+S(\omega)}\right]^{\left[\frac{S(\vartheta)\times S(\omega)}{S(\vartheta)+S(\omega)}\right]}\right] \tag{8}$$

- **The Neighborhood *SS* Entropy**

  If $\psi(\vartheta\omega) = \sqrt{\frac{S(\vartheta)\times S(\omega)}{S(\vartheta)+S(\omega)}}$, then

  $$\sum_{\vartheta\omega\in E(G)} \psi(\vartheta\omega) = \sum_{\vartheta\omega\in E(G)} \sqrt{\frac{S(\vartheta)\times S(\omega)}{S(\vartheta)+S(\omega)}} = SS(G)$$

  Using the definition of Eq. (1) for neighborhood *SS* index results in neighborhood *SS* entropy given by

$$ENT_{NSS(G)} = log(NSS(G)) - \frac{1}{NSS(G)} log\left[\prod_{\vartheta\omega\in E(G)}\left[\sqrt{\frac{S(\vartheta)\times S(\omega)}{S(\vartheta)+S(\omega)}}\right]^{\left[\sqrt{\frac{S(\vartheta)\times S(\omega)}{S(\vartheta)+S(\omega)}}\right]}\right] \tag{9}$$

1.2 Chemical Applicability of Defined Degree-Based Entropies

This section concentrates on framing the linear regression model for the properties viz., boiling point (BP), enthalpy (E), π-electron energy ($\pi - ele$) and molecular weight (MW) of benzene derivatives. They are presented for entropies such as ENT_{SO}, ENT_{GH}, ENT_{HG}, ENT_{SS}, ENT_{NSO}, ENT_{NReZ_1}, ENT_{NReZ_2} and ENT_{NSS}. The properties considered [41–44] in the study have shown a good correlation with the defined entropies.

The ENT_{SO}, ENT_{GH}, ENT_{HG}, ENT_{SS}, ENT_{NSO}, ENT_{NReZ_1}, ENT_{NReZ_2} and ENT_{NSS} are calculated and shown in Table 1.

The linear regression models for BP, E, π-ele and MW are fitted using least squares method for the data presented in Table 1.

Table 1: Experimental values (BP, E, π-ele, MW) of benzenoid hydrocarbons and the corresponding values of ENT_{SO}, ENT_{GH}, ENT_{HG}, ENT_{SS}, ENT_{NSO}, ENT_{NReZ_1}, ENT_{NReZ_2} and ENT_{NSS}

Dervatives of benzene	BP	E	π-ele	MW	ENT_{SO}	ENT_{GH}
Benzene	80.1	75.2	8	78.11	3.683	4.144
Naphthalene	218	141	13.683	128.17	4.576	5.01
Phenanthrene	338	202.7	19.448	178.23	5.265	5.871
Anthracene	340	222.6	19.314	178.23	5.278	5.858
Chrysene	431	271.1	25.192	228.3	5.798	5.951
Benzo[a]anthracene	425	277.1	25.101	228.3	5.803	6.485
Triphenylene	429	275.1	25.275	228.3	5.794	6.51
Tetrcene	440	310.5	25.188	228.3	5.812	6.476
Benzo[a]pyrene	496	296	28.222	252.3	6.084	6.848
Benzo[e]pyrene	493	289.9	28.336	252.3	6.079	6.855
Perylene	497	319.2	28.245	252.3	6.079	6.855
Anthanthrene	547	323	31.253	276.3	6.154	7.133
Benzo[ghi]perylene	542	326.1	31.425	276.3	6.322	7.14
Dibenzi[a,c]anthracene	535	348	30.942	278.3	6.192	6.938
Dibenzo[a,h]anthracene	535	335	30.881	292.4	6.196	6.93
Dibenzo[a,j]anthracene	531	336.3	30.88	281.3	6.196	6.93
Picene	519	336.9	30.943	278.3	6.192	6.938
Coronene	590	296.7	34.572	300.4	6.536	7.384
Dienzo[a,h]pyrene	596	375.6	33.928	302.4	6.417	7.209
Dienzo[a,i]pyrene	594	366	33.954	302.4	6.417	7.209
Dienzo[a,l]pyrene	595	393.3	34.031	302.4	6.414	7.216
Pyrene	393	221.3	22.506	202.25	5.654	6.37
Dervatives of benzene	ENT_{HG}	ENT_{SS}	ENT_{NSO}	ENT_{NReZ_1}	ENT_{NReZ_2}	ENT_{NSS}
Benzene	−0.805	2.154	4.592	−0.862	3.203	−0.304
Naphthalene	−0.594	2.92	5.913	1.482	4.598	4.029
Phenanthrene	−0.247	3.674	5.242	1.94	4.688	4.123
Anthracene	−0.156	3.693	5.998	1.677	4.849	4.2
Chrysene	0.1062	4.13	6.386	1.996	5.237	4.603
Benzo[a]anthracene	0.143	4.138	5.816	2.029	4.986	4.539
Triphenylene	0.149	4.133	6.881	1.982	5.509	4.757
Tetrcene	0.213	4.15	6.706	1.977	5.428	4.714
Benzo[a]pyrene	0.214	4.373	6.333	2.482	5.284	4.763
Benzo[e]pyrene	0.227	4.373	6.432	2.36	5.393	4.822
Perylene	0.227	4.373	6.705	2.23	5.551	4.878
Anthanthrene	0.347	4.589	7.214	2.098	5.926	5.154
Benzo[ghi]perylene	0.347	4.586	6.899	2.217	5.746	5.072
Dibenzi[a,c]anthracene	0.388	4.49	6.785	2.367	5.503	4.973
Dibenzo[a,h]anthracene	0.502	4.493	6.661	2.31	5.554	4.926
Dibenzo[a,j]anthracene	0.502	4.493	6.661	2.31	5.554	4.926
Picene	0.388	4.49	6.959	2.212	5.709	4.999

(Continued)

Table 1 (continued)

Dervatives of benzene	ENT_{HG}	ENT_{SS}	ENT_{NSO}	ENT_{NReZ_1}	ENT_{NReZ_2}	ENT_{NSS}
Coronene	0.49	4.778	7.684	2.236	6.288	5.442
Dienzo[a,h]pyrene	0.599	4.688	6.684	2.436	5.65	5.123
Dienzo[a,i]pyrene	0.599	4.688	6.684	2.436	5.65	5.123
Dienzo[a,l]pyrene	0.609	4.689	6.703	2.526	5.671	5.083
Pyrene	−0.225	3.981	6.433	1.893	5.22	4.566

The models fitted for ENT_{SO} are

$$BP = 190.6\ (\pm 6.276)ENT_{SO} - 655.096\ (\pm 37.014) \tag{10}$$

$$E = 108.097\ (\pm 8.357)ENT_{SO} - 345.434\ (\pm 49.282) \tag{11}$$

$$\pi - ele = 10.080\ (\pm 0.449)ENT_{SO} - 32.197\ (\pm 2.646) \tag{12}$$

$$MW = 86.748\ (\pm 4.116)ENT_{SO} - 266.352\ (\pm 24.272) \tag{13}$$

The models fitted for ENT_{GH} are

$$BP = 160.894\ (\pm 6.565)ENT_{GH} - 593.023\ (\pm 43.342) \tag{14}$$

$$E = 90.611\ (\pm 7.801)ENT_{GH} - 306.043\ (\pm 51.508) \tag{15}$$

$$\pi - ele = 8.521\ (\pm 0.419)ENT_{GH} - 28.997\ (\pm 2.766) \tag{16}$$

$$MW = 73.130\ (\pm 3.996)ENT_{GH} - 237.460\ (\pm 26.384) \tag{17}$$

The models fitted for ENT_{HG} are

$$BP = 331.917\ (\pm 16.403)ENT_{HG} + 401.306\ (\pm 6.781) \tag{18}$$

$$E = 197.177(\pm 9.610)ENT_{HG} + 252.060(\pm 3.973) \tag{19}$$

$$\pi - ele = 17.788(\pm 0.788)ENT_{HG} + 23.625(\pm 0.326) \tag{20}$$

$$MW = 154.499\ (\pm 5.532)ENT_{HG} + 213.819\ (\pm 2.287) \tag{21}$$

The models fitted for ENT_{SS} are

$$BP = 204.078\ (\pm 6.950)ENT_{SS} - 392.055\ (\pm 29.394) \tag{22}$$

$$E = 115.902\ (\pm 8.905)ENT_{SS} - 196.928\ (\pm 37.661) \tag{23}$$

$$\pi - ele = 10.777\ (\pm 0.506)ENT_{SS} - 18.225\ (\pm 2.139) \tag{24}$$

$$MW = 92.772\ (\pm 4.594)ENT_{SS} - 146.175\ (\pm 19.430) \tag{25}$$

The models fitted for ENT_{NSO} are

$$BP = 164.761\ (\pm 23.838)ENT_{NSO} - 604.233\ (\pm 155.021) \tag{26}$$

$$E = 89.087\ (\pm 16.788)ENT_{NSO} - 288.401\ (\pm 109.175) \tag{27}$$

$$\pi - ele = 8.820\ (\pm 1.261)ENT_{NSO} - 30.199\ (\pm 8.200) \tag{28}$$

$$MW = 74.984\ (\pm 11.262)ENT_{NSO} - 243.183\ (\pm 73.241) \tag{29}$$

The models fitted for ENT_{NReZ_1} are

$$BP = 161.292\ (\pm 20.581)ENT_{NReZ_1} + 136.973\ (\pm 43.764) \tag{30}$$

$$E = 92.088\ (\pm 13.555)ENT_{NReZ_1} + 102.544\ (\pm 28.822) \tag{31}$$

$$\pi - ele = 8.263\ (\pm 1.222)ENT_{NReZ_1} + 10.226\ (\pm 2.598) \tag{32}$$

$$MW = 71.638\ (\pm 10.428)ENT_{NReZ_1} + 97.710\ (\pm 22.174) \tag{33}$$

The models fitted for ENT_{NReZ_2} are

$$BP = 194.930\ (\pm 17.009)ENT_{NReZ_2} - 576.413\ (\pm 91.188) \tag{34}$$

$$E = 106.499\ (\pm 14.300)ENT_{NReZ_2} - 279.217\ (\pm 76.661) \tag{35}$$

$$\pi - ele = 10.303\ (\pm 0.960)ENT_{NReZ_2} - 28.006\ (\pm 5.149) \tag{36}$$

$$MW = 88.044\ (\pm 8.732)ENT_{NReZ_2} - 226.952\ (\pm 46.811) \tag{37}$$

The models fitted for ENT_{NSS} are

$$BP = 95.807\ (\pm 13.311)ENT_{NSS} + 24.289(\pm 62.604) \tag{38}$$

$$E = 53.271(\pm 9.070)ENT_{NSS} + 44.738(\pm 42.659) \tag{39}$$

$$\pi - ele = 4.916(\pm 0.775)ENT_{NSS} + 4.417(\pm 3.647) \tag{40}$$

$$MW = 42.370(\pm 6.707)ENT_{NSS} + 48.494(\pm 31.544) \tag{41}$$

Note: The errors associated with the regression coefficients are enclosed with in brackets of Eqs. (10)–(41).

Tables 2 to 9 and Fig. 2 show the r (coefficient of correlation) and RSE (residual standard error) of the above properties using regression models with ENT_{SO}, ENT_{GH}, ENT_{HG}, ENT_{SS}, ENT_{NSO}, ENT_{NReZ_1}, ENT_{NReZ_2} and ENT_{NSS} entropies.

By inspection of Table 2, it shows that ENT_{SO} and BP are highly correlated with $r = 0.989$. Also, ENT_{SO} and E have $r = 0.945$, ENT_{SO} and $\pi - ele$ have $r = 0.981$, ENT_{SO} and MW have $r = 0.978$.

Table 2: The regression models of statistical parameters for ENT_{SO}

Physical properties	r	r^2	*F*	*RSE*	*Significant*
Boiling point	0.989	0.979	922.191	19.257	0.000
Enthalpy	0.945	0.893	167.33	25.64	0.000
$\pi-$ele	0.981	0.962	504.695	1.377	0.000
Molecular weight	0.978	0.957	444.222	12.628	0.000

Table 3: The regression models of statistical parameters for ENT_{GH}

Physical properties	r	r^2	*F*	*RSE*	*Significant*
Boiling point	0.984	0.968	600.698	23.73	0.000
Enthalpy	0.933	0.871	134.901	28.195	0.000
$\pi-$ele	0.977	0.954	413.597	1.514	0.000
Molecular weight	0.971	0.944	334.902	14.442	0.000

Table 4: The regression models of statistical parameters for ENT_{HG}

Physical properties	r	r^2	*F*	*RSE*	*Significant*
Boiling point	0.976	0.953	409.445	28.524	0.000
Enthalpy	0.977	0.955	421.006	16.710	0.000
$\pi-$ele	0.981	0.962	509.755	1.37	0.000
Molecular weight	0.987	0.975	780.104	9.619	0.000

Table 5: The regression models of statistical parameters for ENT_{SS}

Physical properties	r	r^2	*F*	*RSE*	*Significant*
Boiling point	0.989	0.977	862.189	19.901	0.000
Enthalpy	0.946	0.894	169.403	25.498	0.000
$\pi-$ele	0.979	0.958	454.259	1.45	0.000
Molecular weight	0.976	0.953	407.788	13.155	0.000

Table 6: The regression models of statistical parameters for ENT_{NSO}

Physical properties	r	r^2	*F*	*RSE*	*Significant*
Boiling point	0.840	0.705	47.773	71.801	0.000
Enthalpy	0.765	0.585	28.160	50.566	0.000
$\pi-$ele	0.843	0.710	48.922	3.798	0.000
Molecular weight	0.830	0.689	44.329	33.923	0.000

Table 7: The regression models of statistical parameters for ENT_{NReZ_1}

Physical properties	r	r^2	F	RSE	$Significant$
Boiling point	0.869	0.754	61.416	65.51	0.000
Enthalpy	0.835	0.698	46.156	43.144	0.000
$\pi-$ele	0.834	0.696	45.740	3.889	0.000
Molecular weight	0.838	0.702	47.193	33.192	0.000

Table 8: The regression models of statistical parameters for ENT_{NReZ_2}

Physical properties	r	r^2	F	RSE	$Significant$
Boiling point	0.932	0.868	131.336	48.049	0.000
Enthalpy	0.857	0.735	55.469	40.395	0.000
$\pi-$ele	0.923	0.852	115.057	2.713	0.000
Molecular weight	0.914	0.836	101.675	24.666	0.000

Table 9: The regression models of statistical parameters for ENT_{NSS}

Physical properties	r	r^2	F	RSE	$Significant$
Boiling point	0.849	0.721	51.808	69.762	0.000
Enthalpy	0.796	0.633	34.496	47.536	0.000
$\pi-$ele	0.817	0.668	40.193	4.064	0.000
Molecular weight	0.816	0.666	39.912	35.150	0.000

From Table 3, it is observed that ENT_{GH} and BP are are highly correlated with $r = 0.984$. Also, ENT_{GH} and E have $r = 0.933$, ENT_{GH} and $\pi - ele$ have $r = 0.977$, ENT_{GH} and MW have $r = 0.971$.

From Table 4, it is observed that ENT_{HG} and MW highly correlated with $r = 0.987$. Also, ENT_{HG} and BP have $r = 0.976$, ENT_{HG} and E have $r = 0.977$, ENT_{HG} and $\pi - ele$ have $r = 0.981$.

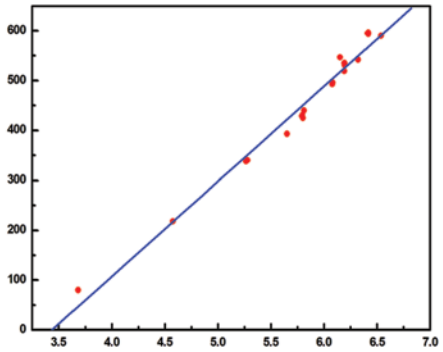
From Table 5, it is observed that ENT_{SS} and BP highly correlated with $r = 0.989$. Also, ENT_{SS} and E have $r = 0.946$, ENT_{SS} and $\pi - ele$ have $r = 0.979$, ENT_{SS} and MW have $r = 0.976$.

From Table 6, it is observed that ENT_{NSO} and $\pi - ele$ highly correlated with $r = 0.843$. Also, ENT_{NSO} and BP have $r = 0.840$, ENT_{NSO} and E have $r = 0.765$, ENT_{NSO} and MW have $r = 0.830$.

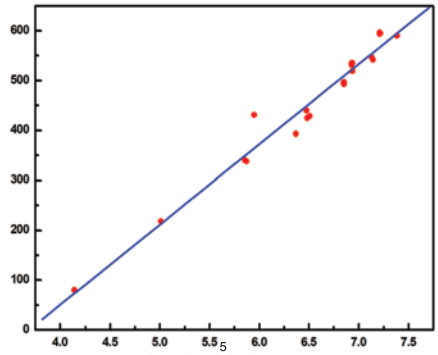
From Table 7, it is observed that ENT_{NReZ_1} and BP highly correlated with $r = 0.869$. Also, ENT_{NReZ_1} and E have $r = 0.835$, ENT_{NReZ_1} and $\pi - ele$ have $r = 0.834$, ENT_{NReZ_1} and MW have $r = 0.838$.

From Table 8, it is observed that ENT_{NReZ_2} and BP highly correlated with $r = 0.932$. Also, ENT_{NReZ_2} and E have $r = 0.857$, ENT_{NReZ_2} and $\pi - ele$ have $r = 0.923$, ENT_{NReZ_2} and MW have $r = 0.914$.

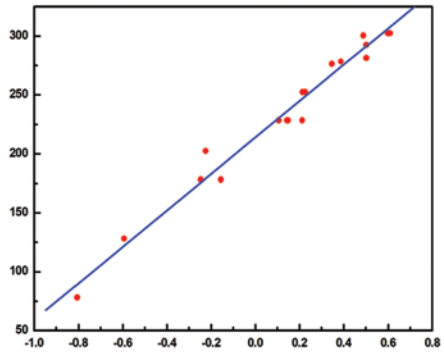
From Table 9, it is observed that ENT_{NSS} and BP highly correlated with $r = 0.849$. Also, ENT_{NSS} and E have $r = 0.796$, ENT_{NSS} and $\pi - ele$ have $r = 0.817$, ENT_{NSS} and MW have $r = 0.816$.



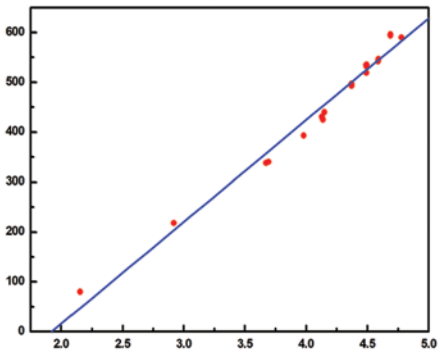
(a) *BP* with ENT_{SO}



(b) *BP* with ENT_{GH}

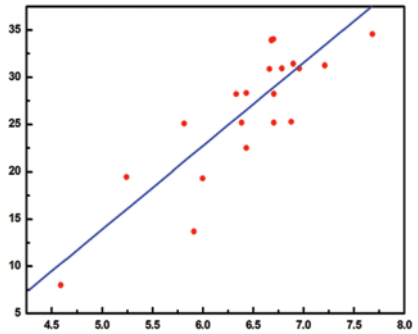


(c) *MW* with ENT_{HG}

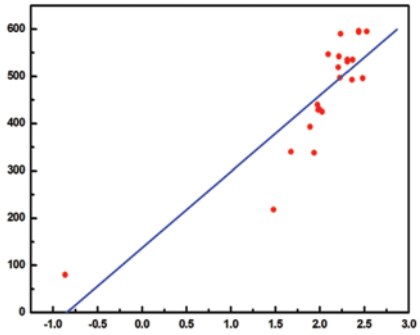


(d) *BP* with ENT_{SS}

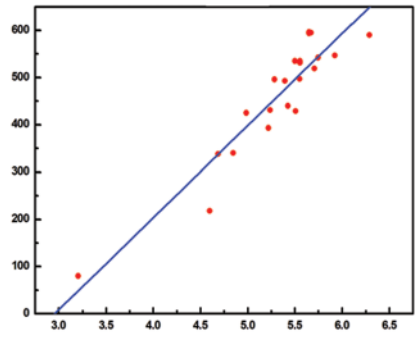
Figure 2: (Continued)



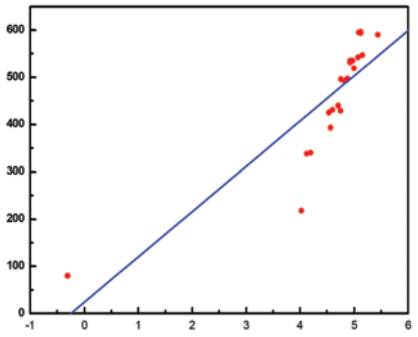
(e) $\pi - ele$ with ENT_{NSO}



(f) BP with ENT_{NReZ_1}



(g) BP with ENT_{NReZ_2}



(h) BP with ENT_{NSS}

Figure 2: Scatter diagram of physical property with entropy descriptor

2 ENT_{SO}, ENT_{GH}, ENT_{HG}, ENT_{SS}, ENT_{NSO}, ENT_{NReZ_1}, ENT_{NReZ_2} and ENT_{NSS} of Graphenylene Molecular Graph

Graphenylene is a cyclic hydrocarbon, where each hexagon has a square adjacent to it. Two such hexagons separated by a square are termed as biphenylene. Chemically, it is a cyclobutadiene ring in between two benzene rings. Graphenylene is modelled as a molecular graph for which the vertices and edges are computed and details are tabulated in Tables 10 and 11 based on degrees and neighborhood degrees of end vertices respectively. From the Fig. 3, the total number of vertices and edges of Graphenylene are $12\,mn$ and $18\,mn - 2\,m - 2\,n$, respectively.

Table 10: The edge partition of molecular graph of $m \times n$ graphenylene structure

$(d(\vartheta), d(\omega))$with $\vartheta\omega \in E(G)$	No. of edges
$(2, 2)$	$(2m + 2n + 2)$
$(2, 3)$	$4m + 4n - 4$
$(3, 3)$	$18mn - 8m - 8n + 2$

Table 11: The edge partition of molecular graph of $m \times n$ graphenylene structure for neighborhood degree based vertices

$(S(\vartheta), S(\omega))$ with $\vartheta\omega \in E(G)$	No. of edges	$(S(\vartheta), S(\omega))$ with $\vartheta\omega \in E(G)$	No. of edges
$(4, 4)$	2	$(8, 8)$	$4m + 4n - 4$
$(4, 5)$	4	$(8, 9)$	4
$(5, 5)$	$2m + 2n - 4$	$(9, 9)$	$8m + 8n - 16$
$(5, 8)$	$18mn - 16m - 16n + 14$	–	–

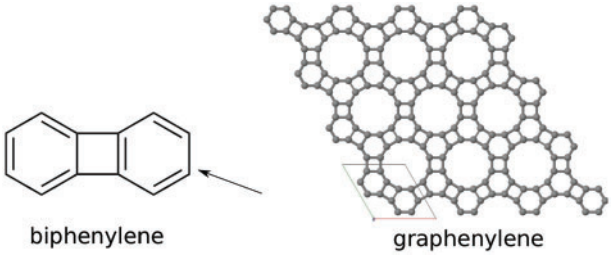


Figure 3: Planar view of 4×4 supercells of biphenylene (graphenylene)

In this section, ENT_{SO}, ENT_{GH}, ENT_{HG}, ENT_{SS}, ENT_{NSO}, ENT_{NReZ_1}, ENT_{NReZ_2} and ENT_{NSS} of graphenylene are computed.

2.1 Results for Graphenylene for Degree Based Vertices

Theorem 2.1. Consider graphenylene structure as a molecular graph G, then the Sombor entropy is:

$$ENT_{SO}(G) = \log(76.368mn - 13.862m - 13.862n - 0.28)$$
$$- \frac{\log\left[(2m+2n+2)\times(\sqrt{8})^{\sqrt{8}}\right]}{(76.368mn - 13.862m - 13.862n - 0.28)} - \frac{\log\left[(4m+4n-4)\times(\sqrt{13})^{\sqrt{13}}\right]}{(76.368mn - 13.862m - 13.862n - 0.28)}$$
$$- \frac{\log\left[(18mn-8m-8n+2)\times(\sqrt{18})^{\sqrt{18}}\right]}{(76.368mn - 13.862m - 13.862n - 0.28)}.$$

Proof. The Sombor entropy and Sombor index are computed as per the above definitions and Table 10.

Then the Sombor index is given by

$SO(G) = 76.368mn - 13.862m - 13.862n - 0.28.$

The Sombor entropy is computed for graphenylene structure using Eq. (2) and Table 10, which results in:

$$ENT_{SO}(G) = log(SO(G)) - \frac{1}{SO(G)} log\left[\prod_{(2,2)\in E_1(G)}\left[\frac{1}{\sqrt{(2)^2+(2)^2}}\right]^{\frac{1}{\sqrt{(2)^2+(2)^2}}}\right.$$
$$\left.\times \prod_{(2,3)\in E_2(G)}\left[\frac{1}{\sqrt{(2)^2+(3)^2}}\right]^{\frac{1}{\sqrt{(2)^2+(3)^2}}} + \prod_{(3,3)\in E_3(G)}\left[\frac{1}{\sqrt{(3)^2+(3)^2}}\right]^{\frac{1}{\sqrt{(3)^2+(3)^2}}}\right]$$
$$ENT_{SO}(G) = log(SO(G))$$
$$- \frac{1}{SO(G)}\log\left[\left[(2m+2n+2)\times(\sqrt{8})^{\sqrt{8}}\right]\times\left[(4m+4n-4)\times(\sqrt{13})^{\sqrt{13}}\right]\right.$$
$$\left.\times\left[(18mn-8m-8n+2)\times(\sqrt{18})^{\sqrt{18}}\right]\right]$$
$$ENT_{SO}(G) = \log(76.368mn - 13.862m - 13.862n - 0.28)$$
$$- \frac{\log\left[(2m+2n+2)\times(\sqrt{8})^{\sqrt{8}}\right]}{(76.368mn - 13.862m - 13.862n - 0.28)} - \frac{\log\left[(4m+4n-4)\times(\sqrt{13})^{\sqrt{13}}\right]}{(76.368mn - 13.862m - 13.862n - 0.28)}$$
$$- \frac{\log\left[(18mn-8m-8n+2)\times(\sqrt{18})^{\sqrt{18}}\right]}{(76.368mn - 13.862m - 13.862n - 0.28)}.$$

Theorem 2.2. Consider graphenylene structure as a molecular graph G, then the GH entropy is:

$$ENT_{GH}(G) = \log(162mn - 39.504m - 39.504n + 1.504)$$
$$- \frac{\log\left[(2m+2n+2)\times(4)^4\right]}{(162mn - 39.504m - 39.504n + 1.504)} - \frac{\log\left[(4m+4n-4)\times(6.124)^{6.124}\right]}{(162mn - 39.504m - 39.504n + 1.504)}$$
$$- \frac{\log\left[(18mn-8m-8n+2)\times(9)^9\right]}{(162mn - 39.504m - 39.504n + 1.504)}.$$

Proof. The *GH* entropy and *GH* index are computed as per the above definitions and Table 10.

Then, the *GH* index is given by

$GH(G) = 162mn - 39.504m - 39.504n + 1.504.$

The *GH* entropy is calculated for graphenylene structure using Eq. (3) and Table 10, results in:

$$ENT_{GH}(G) = log(GH(G)) - \frac{1}{GH(G)} log\left[\prod_{(2,2)\in E_1(G)}\left[\frac{(2+2)(\sqrt{2\times 2})}{2}\right]^{\frac{(2+2)(\sqrt{2\times 2})}{2}} \times \prod_{(2,3)\in E_2(G)}\left[\frac{(2+3)(\sqrt{2\times 3})}{2}\right]^{\frac{(2+3)(\sqrt{2\times 3})}{2}} \times \prod_{(3,3)\in E_3(G)}\left[\frac{(3+3)(\sqrt{3\times 3})}{2}\right]^{\frac{(3+3)(\sqrt{3\times 3})}{2}}\right]$$

$$ENT_{GH}(G) = log(GH(G)) - \frac{1}{GH(G)} \log\left[\left[(2m+2n+2)\times(4)^4\right]\times\left[(4m+4n-4)\times(6.124)^{6.124}\right] \times[(18mn-8m-8n+2)\times(9)^9]\right]$$

$$ENT_{GH}(G) = \log(162mn - 39.504m - 39.504n + 1.504) - \frac{\log[(2m+2n+2)\times(4)^4]}{(162mn-39.504m-39.504n+1.504)} - \frac{\log[(4m+4n-4)\times(6.124)^{6.124}]}{(162mn-39.504m-39.504n+1.504)} - \frac{\log[(18mn-8m-8n+2)\times(9)^9]}{(162mn-39.504m-39.504n+1.504)}.$$

Theorem 2.3. Consider graphenylene structure as a molecular graph *G*, then the *HG* entropy is:

$$ENT_{HG}(G) = \log(1.998mn + 0.264m + 0.264\,n + 0.07) - \frac{\log[(2m+2n+2)\times(0.25)^{0.25}]}{(1.998mn+0.264m+0.264n+0.07)} - \frac{\log[(4m+4n-4)\times(0.163)^{0.163}]}{(1.998mn+0.264m+0.264n+0.07)} - \frac{\log[(18mn-8m-8n+2)\times(0.111)^{0.111}]}{(1.998mn+0.264m+0.264n+0.07)}.$$

Proof. The *HG* entropy and *HG* index are computed as per the above definitions and Table 10.

Then, the *HG* index is given by

$HG(G) = 1.998mn + 0.264m + 0.264n + 0.07.$

The HG entropy is calculated for graphenylene structure using Eq. (4) and Table 10, results in:

$$ENT_{HG}(G) = log(HG(G)) - \frac{1}{HG(G)} log\left[\prod_{(2,2)\in E_1(G)}\left[\frac{2}{(2+2)(\sqrt{2\times 2})}\right]^{\frac{2}{(2+2)(\sqrt{2\times 2})}} \times \prod_{(2,3)\in E_2(G)}\left[\frac{2}{(2+3)(\sqrt{2\times 3})}\right]^{\frac{2}{(2+3)(\sqrt{2\times 3})}} \times \prod_{(3,3)\in E_3(G)}\left[\frac{2}{(3+3)(\sqrt{3\times 3})}\right]^{\frac{2}{(3+3)(\sqrt{3\times 3})}}\right]$$

$$ENT_{HG}(G) = log(HG(G))$$

$$-\frac{1}{HG(G)}\log\left[\left[(2m+2n+2)\times(0.25)^{0.25}\right]\times\left[(4m+4n-4)\times(0.163)^{0.163}\right]\right.$$
$$\left.\times\left[(18mn-8m-8n+2)\times(0.111)^{0.111}\right]\right]$$
$$ENT_{HG}(G)=\log(1.998mn+0.264m+0.264n+0.07)$$
$$-\frac{\log\left[(2m+2n+2)\times(0.25)^{0.25}\right]}{(1.998mn+0.264m+0.264n+0.07)}-\frac{\log\left[(4m+4n-4)\times(0.163)^{0.163}\right]}{(1.998mn+0.264m+0.264n+0.07)}$$
$$-\frac{\log\left[(18mn-8m-8n+2)\times(0.111)^{0.111}\right]}{(1.998mn+0.264m+0.264n+0.07)}.$$

Theorem 2.4. Consider graphenylene structure as a molecular graph G, then the SS entropy is:

$$ENT_{SS}(G)=\log(22.05mn-3.42m-3.42n+0.07)$$
$$-\frac{\log\left[(2m+2n+2)\times(1)^{1}\right]}{(22.05mn-3.42m-3.42n+0.07)}-\frac{\log\left[(4m+4n-4)\times(1.095)^{1.095}\right]}{(22.05mn-3.42m-3.42n+0.07)}$$
$$-\frac{\log\left[(18mn-8m-8n+2)\times(1.225)^{1.225}\right]}{(22.05mn-3.42m-3.42n+0.07)}.$$

Proof. The SS entropy and SS index are computed as per the above definitions and Table 10.

Then, the SS index is given by

$SS(G)=22.05mn-3.42m-3.42n+0.07.$

The SS entropy is calculated for graphenylene structure using Eq. (5) and Table 10, which results in:

$$ENT_{SS}(G)=log(SS(G))-\frac{1}{SS(G)}log\left[\prod_{(2,2)\in E_1(G)}\left[\sqrt{\frac{2\times2}{2+2}}\right]^{\sqrt{\frac{2\times2}{2+2}}}\right.$$
$$\left.\times\prod_{(2,3)\in E_2(G)}\left[\sqrt{\frac{2\times3}{2+3}}\right]^{\sqrt{\frac{2\times3}{2+3}}}\times\prod_{(3,3)\in E_3(G)}\left[\sqrt{\frac{3\times3}{3+3}}\right]^{\sqrt{\frac{3\times3}{3+3}}}\right]$$
$$ENT_{SS}(G)=log(SS(G))$$
$$-\frac{1}{SS(G)}\log\left[\left[(2m+2n+2)\times(1)^{1}\right]\times\left[(4m+4n-4)\times(1.095)^{1.095}\right]\right.$$
$$\left.\times\left[(18mn-8m-8n+2)\times(1.225)^{1.225}\right]\right]$$
$$ENT_{SS}(G)=\log(22.05mn-3.42m-3.42n+0.07)$$
$$-\frac{\log\left[(2m+2n+2)\times(1)^{1}\right]}{(22.05mn-3.42m-3.42n+0.07)}-\frac{\log\left[(4m+4n-4)\times(1.095)^{1.095}\right]}{(22.05mn-3.42m-3.42n+0.07)}$$
$$-\frac{\log\left[(18mn-8m-8n+2)\times(1.225)^{1.225}\right]}{(22.05mn-3.42m-3.42n+0.07)}.$$

2.2 *Results for Graphenylene Using Neighbourhood Degree of End Vertices*

Theorem 2.5. Consider graphenylene structure as a molecular graph G, then the neighborhood Sombor entropy is:

$$ENT_{NSO}(G) = \log(229.102mn - 55.436m - 55.436n + 1.686)$$
$$- \frac{\log\left[(2) \times (\sqrt{32})^{\sqrt{32}}\right]}{(229.102mn - 55.436m - 55.436n + 1.686)} - \frac{\log\left[(4) \times (\sqrt{41})^{\sqrt{41}}\right]}{(229.102mn - 55.436m - 55.436n + 1.686)}$$
$$- \frac{\log\left[(2m + 2n - 4) \times (\sqrt{50})^{\sqrt{50}}\right]}{(229.102mn - 55.436m - 55.436n + 1.686)} - \frac{\log\left[(4m + 4n - 4) \times (\sqrt{89})^{\sqrt{89}}\right]}{(229.102mn - 55.436m - 55.436n + 1.686)}$$
$$- \frac{\log\left[(4) \times (\sqrt{28})^{\sqrt{28}}\right]}{(229.102mn - 55.436m - 55.436n + 1.686)} - \frac{\log\left[(8m + 8n - 16) \times (\sqrt{145})^{\sqrt{145}}\right]}{(229.102mn - 55.436m - 55.436n + 1.686)}$$
$$- \frac{\log\left[(18mn - 16m - 16n + 14) \times (\sqrt{162})^{\sqrt{162}}\right]}{(229.102mn - 55.436m - 55.436n + 1.686)}.$$

Proof. The neighborhood Sombor entropy and neighborhood Sombor index are computed as per the above definitions and Table 11.

Then, the neighborhood Sombor index is given by

$NSO(G) = 229.102mn - 55.436m - 55.436n + 1.686.$

The neighborhood Sombor entropy is calculated for graphenylene structure using Eq. (6) and Table 11, which results in:

$$ENT_{NSO}(G) = log(NSO(G)) - \frac{1}{NSO(G)} log\left[\prod_{(4,4)\in E_1(G)}\left[\sqrt{(4)^2+(4)^2}\right]^{\sqrt{(4)^2+(4)^2}}\right.$$
$$\times \prod_{(4,5)\in E_2(G)}\left[\sqrt{(4)^2+(5)^2}\right]^{\sqrt{(4)^2+(5)^2}} \times \prod_{(5,5)\in E_3(G)}\left[\sqrt{(5)^2+(5)^2}\right]^{\sqrt{(5)^2+(5)^2}}$$
$$\times \prod_{(5,8)\in E_2(G)}\left[\sqrt{(5)^2+(8)^2}\right]^{\sqrt{(5)^2+(8)^2}} \times \prod_{(8,8)\in E_3(G)}\left[\sqrt{(8)^2+(8)^2}\right]^{\sqrt{(8)^2+(8)^2}}$$
$$\left.\times \prod_{(8,9)\in E_4(G)}\left[\sqrt{(8)^2+(9)^2}\right]^{\sqrt{(8)^2+(9)^2}} \times \prod_{(9,9)\in E_4(G)}\left[\sqrt{(9)^2+(9)^2}\right]^{\sqrt{(9)^2+(9)^2}}\right]$$
$$ENT_{NSO}(G) = log(NSO(G)) - \frac{1}{NSO(G)} \log\left[\left[(2) \times (\sqrt{32})^{\sqrt{32}}\right] \times \left[(4) \times (\sqrt{41})^{\sqrt{41}}\right]\right.$$
$$\times \left[(2m + 2n - 4) \times (\sqrt{50})^{\sqrt{50}}\right] \times [(4m + 4n - 4) \times (\sqrt{89})^{\sqrt{89}}] \times \left[(4) \times (\sqrt{128})^{\sqrt{128}}\right]$$
$$\left.\times \left[(8m + 8n - 16) \times (\sqrt{145})^{\sqrt{145}}\right] \times \left[(18mn - 16m - 16n + 14) \times (\sqrt{162})^{\sqrt{162}}\right]\right]$$
$$ENT_{NSO}(G) = \log(229.102mn - 55.436m - 55.436n + 1.686)$$

$$-\frac{\log\left[(2)\times(\sqrt{32})^{\sqrt{32}}\right]}{(229.102mn-55.436m-55.436n+1.686)}-\frac{\log\left[(4)\times(\sqrt{41})^{\sqrt{41}}\right]}{(229.102mn-55.436m-55.436n+1.686)}$$
$$-\frac{\log\left[(2m+2n-4)\times(\sqrt{50})^{\sqrt{50}}\right]}{(229.102mn-55.436m-55.436n+1.686)}-\frac{\log\left[(4m+4n-4)\times(\sqrt{89})^{\sqrt{89}}\right]}{(229.102mn-55.436m-55.436n+1.686)}$$
$$-\frac{\log\left[(4)\times(\sqrt{28})^{\sqrt{28}}\right]}{(229.102mn-55.436m-55.436n+1.686)}-\frac{\log\left[(8m+8n-16)\times(\sqrt{145})^{\sqrt{145}}\right]}{(229.102mn-55.436m-55.436n+1.686)}$$
$$-\frac{\log\left[(18mn-16m-16n+14)\times(\sqrt{162})^{\sqrt{162}}\right]}{(229.102mn-55.436m-55.436n+1.686)}.$$

Theorem 2.6. Consider graphenylene structure as a molecular graph G, then $NReZ_1$ entropy is:

$$ENT_{NReZ_1}(G)=\log(3.966mn+0.436mn+0.436n+0.232)$$
$$-\frac{\log[(2)\times(0.5)^{0.5}]}{(3.966mn+0.436mn+0.436n+0.232)}-\frac{\log[(4)\times(0.45)^{0.45}]}{(3.966mn+0.436mn+0.436n+0.232)}$$
$$-\frac{\log[(2m+2n-4)\times(0.4)^{0.4}]}{(3.966mn+0.436mn+0.436n+0.232)}-\frac{\log[(4m+4n-4)\times(0.325)^{0.325}]}{(3.966mn+0.436mn+0.436n+0.232)}$$
$$-\frac{\log[(4)\times(0.25)^{0.25}]}{(3.966mn+0.436mn+0.436n+0.232)}-\frac{\log[(8m+8n-16)\times(0.236)^{0.236}]}{(3.966mn+0.436mn+0.436n+0.232)}$$
$$-\frac{\log[(18mn-16m-16n+14)\times(0.222)^{0.222}]}{(3.966mn+0.436mn+0.436n+0.232)}.$$

Proof.

The $NReZ_1$ entropy and $NReZ_1$ index are computed as per the above definitions and Table 11.

Then, the $NReZ_1$ index is given by

$NReZ_1(G)=3.966mn+0.436mn+0.436n+0.232.$

The $NReZ_1$ entropy is calculated for graphenylene using Eq. (7) and Table 11, which results in:

$$ENT_{NReZ_1}(G)=log(NReZ_1(G))-\frac{1}{NReZ_1(G)}log\left[\prod_{(4,4)\in E_1(G)}\left[\frac{4+4}{4\times4}\right]^{\frac{4+4}{4\times4}}\right.$$
$$\times\prod_{(4,5)\in E_2(G)}\left[\frac{4+5}{4\times5}\right]^{\frac{4+5}{4\times5}}\times\prod_{(5,5)\in E_3(G)}\left[\frac{5+5}{5\times5}\right]^{\frac{5+5}{5\times5}}\times\prod_{(5,8)\in E_2(G)}\left[\frac{5+8}{5\times8}\right]^{\frac{5+8}{5\times8}}$$
$$\left.\times\prod_{(8,8)\in E_3(G)}\left[\frac{8+8}{8\times8}\right]^{\frac{8+8}{8\times8}}\times\prod_{(8,9)\in E_4(G)}\left[\frac{8+9}{8\times9}\right]^{\frac{8+9}{8\times9}}\times\prod_{(9,9)\in E_4(G)}\left[\frac{9+9}{9\times9}\right]^{\frac{9+9}{9\times9}}\right]$$

$$ENT_{NReZ_1}(G)=log(NReZ_1(G))-\frac{1}{NReZ_1(G)}\log\left[\left[(2)\times(0.5)^{0.5}\right]\times\left[(4)\times(0.45)^{0.45}\right]\right.$$
$$\left.\times\left[(2m+2n-4)\times(0.4)^{0.4}\right]\times\left[(4m+4n-4)\times(0.325)^{0.325}\right]\times\left[(4)\times(0.25)^{0.25}\right]\right.$$

$$\times\left[(8m+8n-16)\times(0.236)^{0.236}\right]\times\left[(18mn-16m-16n+14)\times(0.222)^{0.222}\right]]$$

$$ENT_{NReZ_1}(G)=\log(3.966mn+0.436mn+0.436n+0.232)$$
$$-\frac{\log[(2)\times(0.5)^{0.5}]}{(3.966mn+0.436mn+0.436n+0.232)}-\frac{\log[(4)\times(0.45)^{0.45}]}{(3.966mn+0.436mn+0.436n+0.232)}$$
$$-\frac{\log[(2m+2n-4)\times(0.4)^{0.4}]}{(3.966mn+0.436mn+0.436n+0.232)}-\frac{\log[(4m+4n-4)\times(0.325)^{0.325}]}{(3.966mn+0.436mn+0.436n+0.232)}$$
$$-\frac{\log[(4)\times(0.25)^{0.25}]}{(3.966mn+0.436mn+0.436n+0.232)}-\frac{\log[(8m+8n-16)\times(0.236)^{0.236}]}{(3.966mn+0.436mn+0.436n+0.232)}$$
$$-\frac{\log[(18mn-16m-16n+14)\times(0.222)^{0.222}]}{(3.966mn+0.436mn+0.436n+0.232)}.$$

Theorem 2.7. Consider graphenylene structure as a molecular graph G, then $NReZ_2$ entropy is:

$$ENT_{NReZ_2}(G)=\log(81mn-20.812m-20.812n+1.82)$$
$$-\frac{\log[(2)\times(2)^2]}{(81mn-20.812m-20.812n+1.82)}-\frac{\log[(4)\times(2.222)^{2.222}]}{(81mn-20.812m-20.812n+1.82)}$$
$$-\frac{\log[(2m+2n-4)\times(2.5)^{2.5}]}{(81mn-20.812m-20.812n+1.82)}-\frac{\log[(4m+4n-4)\times(3.077)^{3.077}]}{(81mn-20.812m-20.812n+1.82)}$$
$$-\frac{\log[(4)\times(4)^4]}{(81mn-20.812m-20.812n+1.82)}-\frac{\log[(8m+8n-16)\times(4.235)^{4.235}]}{(81mn-20.812m-20.812n+1.82)}$$
$$-\frac{\log[(18mn-16m-16n+14)\times(4.5)^{4.5}]}{(81mn-20.812m-20.812n+1.82)}.$$

Proof. The $NReZ_2$ entropy and $NReZ_2$ index are computed as per the above definitions and Table 11.

Then, the $NReZ_2$ index is given by

$NReZ_2(G)=3.966mn+0.436mn+0.436n+0.232.$

The $NReZ_2$ entropy is calculated for graphenylene using Eq. (8) and Table 11, which results in:

$$ENT_{NReZ_2}(G)=log(NReZ_2(G))-\frac{1}{NReZ_2(G)}log\left[\prod_{(4,4)\in E_1(G)}\left[\frac{4\times4}{4+4}\right]^{\frac{4\times4}{4+4}}\right.$$
$$\times\prod_{(4,5)\in E_2(G)}\left[\frac{4\times5}{4+5}\right]^{\frac{4\times5}{4+5}}\times\prod_{(5,5)\in E_3(G)}\left[\frac{5\times5}{5+5}\right]^{\frac{5\times5}{5+5}}\times\prod_{(5,8)\in E_2(G)}\left[\frac{5\times8}{5+8}\right]^{\frac{5\times8}{5+8}}$$
$$\left.\times\prod_{(8,8)\in E_3(G)}\left[\frac{8\times8}{8+8}\right]^{\frac{8\times8}{8+8}}\times\prod_{(8,9)\in E_4(G)}\left[\frac{8\times9}{8+9}\right]^{\frac{8\times9}{8+9}}\times\prod_{(9,9)\in E_4(G)}\left[\frac{9\times9}{9+9}\right]^{\frac{9\times9}{9+9}}\right]$$

$$ENT_{NReZ_2}(G)=log(NReZ_2(G))-\frac{1}{NReZ_2(G)}\log\left[[(2)\times(2)^2]\times[(4)\times(2.222)^{2.222}]\right.$$

$$\times\left[(2m+2n-4)\times(2.5)^{2.5}\right]\times\left[(4m+4n-4)\times(3.077)^{3.077}\right]\times\left[(4)\times(4)^{4}\right]$$
$$\times\left[(8m+8n-16)\times(4.235)^{4.235}\right]\times\left[(18mn-16m-16n+14)\times(4.5)^{4.5}\right]]$$
$$ENT_{NReZ_2}(G)=\log(81mn-20.812m-20.812n+1.82)$$
$$-\frac{\log[(2)\times(2)^{2}]}{(81mn-20.812m-20.812n+1.82)}-\frac{\log[(4)\times(2.222)^{2.222}]}{(81mn-20.812m-20.812n+1.82)}$$
$$-\frac{\log[(2m+2n-4)\times(2.5)^{2.5}]}{(81mn-20.812m-20.812n+1.82)}-\frac{\log[(4m+4n-4)\times(3.077)^{3.077}]}{(81mn-20.812m-20.812n+1.82)}$$
$$-\frac{\log[(4)\times(4)^{4}]}{(81mn-20.812m-20.812n+1.82)}-\frac{\log[(8m+8n-16)\times(4.235)^{4.235}]}{(81mn-20.812m-20.812n+1.82)}$$
$$-\frac{\log[(18mn-16m-16n+14)\times(4.5)^{4.5}]}{(81mn-20.812m-20.812n+1.82)}.$$

Theorem 2.8. Consider graphenylene structure as a molecular graph G, then neighborhood SS entropy is:

$$ENT_{NSS}(G)=\log(38.18mn-7.298m-7.298n+0.221)$$
$$-\frac{\log[(2)\times(1.414)^{1.414}]}{(38.18mn-7.298m-7.298n+0.221)}-\frac{\log[(4)\times(1.491)^{1.491}]}{(38.18mn-7.298m-7.298n+0.221)}$$
$$-\frac{\log[(2m+2n-4)\times(1.581)^{1.581}]}{(38.18mn-7.298m-7.298n+0.221)}-\frac{\log[(4m+4n-4)\times(1.754)^{1.754}]}{(38.18mn-7.298m-7.298n+0.221)}$$
$$-\frac{\log[(4)\times(2)^{2}]}{(38.18mn-7.298m-7.298n+0.221)}-\frac{\log[(8m+8n-16)\times(2.058)^{2.058}]}{(38.18mn-7.298m-7.298n+0.221)}$$
$$-\frac{\log[(18mn-16m-16n+14)\times(2.121)^{2.121}]}{(38.18mn-7.298m-7.298n+0.221)}.$$

Proof. The neighborhood SS entropy and neighborhood SS index are computed as per the above definitions and Table 11.

Then, the neighborhood SS index is given by

$NSS(G)=38.18mn-7.298m-7.298n+0.221.$

The neighborhood SS entropy is calculated for graphenylene structure using Eq. (9) and Table 11, which results in:

$$ENT_{NSS}(G)=log(NSS(G))-\frac{1}{NSS(G)}log\left[\prod_{(4,4)\in E_1(G)}\left[\sqrt{\frac{4\times4}{4+4}}\right]^{\sqrt{\frac{4\times4}{4+4}}}\right.$$
$$\times\prod_{(4,5)\in E_2(G)}\left[\sqrt{\frac{4\times5}{4+5}}\right]^{\sqrt{\frac{4\times5}{4+5}}}\times\prod_{(5,5)\in E_3(G)}\left[\sqrt{\frac{5\times5}{5+5}}\right]^{\sqrt{\frac{5\times5}{5+5}}}\times\prod_{(5,8)\in E_2(G)}\left[\sqrt{\frac{5\times8}{5+8}}\right]^{\sqrt{\frac{5\times8}{5+8}}}$$

$$\times \prod_{(8,8)\in E_3(G)} \left[\sqrt{\frac{8\times 8}{8+8}}\right]^{\sqrt{\frac{8\times 8}{8+8}}} \times \prod_{(8,9)\in E_4(G)} \left[\sqrt{\frac{8\times 9}{8+9}}\right]^{\sqrt{\frac{8\times 9}{8+9}}} \times \prod_{(9,9)\in E_4(G)} \left[\sqrt{\frac{9\times 9}{9+9}}\right]^{\sqrt{\frac{9\times 9}{9+9}}}\Bigg]$$

$$ENT_{NSS}(G) = log(NSS(G)) - \frac{1}{NSS(G)} \log\big[[(2)\times(1.414)^{1.414}]\times[(4)\times(1.491)^{1.491}]$$
$$\times[(2m+2n-4)\times(1.581)^{1.581}]\times[(4m+4n-4)\times(1.754)^{1.754}]\times[(4)\times(2)^2]$$
$$\times[(8m+8n-16)\times(2.058)^{2.058}]\times[(18mn-16m-16n+14)\times(2.121)^{2.121}]\big]$$

$$ENT_{NSS}(G) = \log(38.18mn - 7.298m - 7.298n + 0.221)$$
$$- \frac{\log[(2)\times(1.414)^{1.414}]}{(38.18mn-7.298m-7.298n+0.221)} - \frac{\log[(4)\times(1.491)^{1.491}]}{(38.18mn-7.298m-7.298n+0.221)}$$
$$- \frac{\log[(2m+2n-4)\times(1.581)^{1.581}]}{(38.18mn-7.298m-7.298n+0.221)} - \frac{\log[(4m+4n-4)\times(1.754)^{1.754}]}{(38.18mn-7.298m-7.298n+0.221)}$$
$$- \frac{\log[(4)\times(2)^2]}{(38.18mn-7.298m-7.298n+0.221)} - \frac{\log[(8m+8n-16)\times(2.058)^{2.058}]}{(38.18mn-7.298m-7.298n+0.221)}$$
$$- \frac{\log[(18mn-16m-16n+14)\times(2.121)^{2.121}]}{(38.18mn-7.298m-7.298n+0.221)}.$$

3 Conclusion

This work is dedicated to defining and discussing the chemical applicability of ENT_{SO}, ENT_{GH}, ENT_{HG}, ENT_{SS}, ENT_{NSO}, ENT_{NReZ_1}, ENT_{NReZ_2} and ENT_{NSS} for a few properties of by-products of benzene molecules by applying regression models and computing entropy descriptors of graphenylene structure. It is observed from the above study that the graph entropies considered have proved to be correlated well with the four physical properties mentioned in this work. The following are the observations made from the study. The ENT_{SO} has a high positive correlation against BP with $r = 0.989$. The ENT_{GH} has a high positive correlation against BP with $r = 0.984$. The ENT_{HG} has a high positive correlation against MW with $r = 0.987$. There is a high positive correlation between ENT_{SS} against BP with $r = 0.989$. The ENT_{NSO} has a high positive correlation against $\pi - ele$ with $r = 0.843$. The ENT_{NReZ_1} has a high positive correlation with BP having $r = 0.869$. The ENT_{NReZ_2} has a high positive correlation with BP with $r = 0.932$. The ENT_{NSS} has a high positive correlation against BP with $r = 0.849$.

There has been a remarkable increase in the applications of graphenylene as it has distinguished mechanical, electrical, and thermal properties. This study provides a way for researchers to study physico-chemical and biological properties of various compounds associated with degree-based entropies.

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