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Computational Analysis of Energy, Closeness Energy, and Topological Connectivity in Benzenoid Hydrocarbons [*]

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ABSTRACT: Benzenoid hydrocarbons are widely studied molecular structures due to their unique topological and chemical properties. This research investigates their structural characteristics by evaluating energy, closeness energy, and a range of distance, degree, and eccentricity-based topological indices. The study focuses on the molecular graphs of 22 benzenoid hydrocarbons by aiming to evaluate how energy, closeness energy, and related topological indices can be used to describe structural properties and establish quantitative relationships with physicochemical data. In addition to deriving analytical expressions and performing computational evaluations, we develop regression models to link energy and closeness energy with selected topological indices and intrinsic physicochemical properties. Unlike previous studies that emphasize only tabulated values, our work demonstrates the predictive potential of combining spectral and topological measures, with closeness energy, providing additional insight into the structural characteristics of benzenoid hydrocarbons. The findings provide a clearer understanding of benzenoid structures and contribute to advancing applications of graph-based methods in molecular graph theory, cheminformatics, and materials science.

Keywords: Molecular graph, distance, graph energies, benzenoid hydrocarbons.

Contents

1. Introduction

Chemical graph theory is a specialized branch of mathematical chemistry that applies graph-theoretic principles to model and analyze molecular structures. By representing molecules as graphs, this field provides valuable insights into their structural, electronic, and thermodynamic properties. It finds applications in molecular stability analysis, drug design, and nanotechnology. A molecular or chemical graph is a simple, finite graph in which atoms are represented by vertices and chemical bonds by edges.

Graph theory has become a fundamental tool for exploring molecular structures, with topological indices playing a crucial role in connecting molecular architecture to physicochemical properties. The growing demand for efficient and accurate computational models in chemistry has led to the development of graph-based descriptors that can reliably predict structural and thermodynamic characteristics. These descriptors simplify complex molecular systems while preserving predictive accuracy by encoding atomic interactions within molecular frameworks.

Topological indices contribute significantly to quantitative structure–property relationships (QSPRs) and quantitative structure–activity relationships (QSARs), offering a systematic means to understand physicochemical features without the need for extensive experimental analysis. By expressing molecular connectivity in numerical terms, these indices assist in estimating properties such as solubility, reactivity,

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stability, and biological activity. Their predictive capabilities are especially valuable in molecular design across fields such as drug development, environmental modeling, and materials science, where optimizing molecular features is essential [19].

Topological indices are categorized based on the types of graph parameters involved in their formulation. One such category is eigenvalue-based topological indices, which are defined using the eigenvalues of matrices associated with the graph. These matrices can include the adjacency matrix, Laplacian matrix, or distance matrix, among others.

Computational methods based on graph-theoretic descriptors provide an efficient alternative to traditional experimental techniques, which are often labor-intensive and resource-intensive. By leveraging these indices, researchers can gain deeper insights into molecular behavior, facilitating the prediction of key thermodynamic parameters such as boiling point (BP), entropy (S), enthalpy of formation (ΔH_f), logarithm of the partition coefficient (log P), and molecular connectivity indices. The ability to model these properties computationally strengthens the understanding of molecular interactions and structural stability, leading to advancements in applied chemistry and molecular engineering. As research continues to evolve, the integration of graph-theoretic methodologies with computational chemistry promises to enhance predictive modeling, making it a valuable asset for modern chemical and materials sciences [24].

Benzenoid hydrocarbons, composed of fused benzene rings, are among the most studied classes of aromatic compounds due to their stability, electronic delocalization, and occurrence in numerous natural and synthetic materials. These structures are essential in organic chemistry and are widely used in materials science, molecular electronics, and environmental chemistry. The aromatic nature of benzenoid hydrocarbons contributes to their characteristic stability and reactivity patterns, making them ideal candidates for graph-theoretic investigations.

The structural characteristics of benzenoid hydrocarbons can be effectively examined using topological indices, which provide numerical representations of molecular features. Energy indices quantify electronic stability, while distance, degree, and eccentricity based indices capture various aspects of molecular connectivity and branching. These indices are widely applied to evaluate molecular complexity and predict chemical and physical behaviors.

Recent studies have emphasized the importance of spectral and distance-based topological indices in chemical graph theory. Kumar et al. [21] investigated eigenvalue-based descriptors such as graph energy and the Estrada index for polycyclic aromatic hydrocarbons, showing strong correlations with classical indices and physicochemical properties. Similarly, recent work on benzenoid hydrocarbons highlighted the role of distance-based invariants in capturing structural features related to stability and reactivity [2]. These contributions confirm the relevance of both spectral and distance-based measures, while also indicating the need for integrated approaches that combine multiple descriptors for predictive modeling.

In addition, Hayat et al. have contributed significantly to the development and application of graph-based indices in diverse contexts. For example, Hayat and Imran [16] analyzed topological properties of nanocones, while Khan et al. [20] extended graph-theoretic methods to neural networks. More recently, Hayat et al. [18] demonstrated the predictive potential of eigenvalue-based indices for thermodynamic properties of polycyclic aromatic hydrocarbons, and Hayat and Asmat [17] investigated sharp bounds on Zagreb indices with applications to QSPR modeling. These studies highlight both the breadth and predictive relevance of graph-theoretic descriptors across chemical and computational domains.

Graph-theoretic methods have also found applications beyond chemistry, including areas such as the Internet of Things (IoT) [4], communication networks [32], computing systems [15], and distributed computing [27]. These diverse applications highlight the versatility of graph-based approaches and further motivate their use in analyzing molecular structures.

This study focuses on the molecular graphs of various benzenoid hydrocarbons. It evaluates a set of topological indices including energy, closeness energy, and several distance, degree and eccentricity-based descriptors. Analytical derivations and computational evaluations are carried out to explore patterns of molecular stability and connectivity. The insights gained from this study offer a deeper understanding of the topological characteristics of benzenoid hydrocarbons and provide a useful reference for future work in molecular graph theory and cheminformatics.

Let $G = (V, E)$ be a molecular graph with $|V| = p$ and $|E| = q$. For an edge xy, we call x and y the end vertices of xy. For a vertex $x \in V(G)$, the open neighborhood of x is the set $N(x) = \{y \in V(G) : xy \in$

$E(G)\}$, and the closed neighborhood of x is $N[x] = N(x) \cup \{x\}$. The degree of a vertex $x \in V(G)$, denoted by d_x, is $|N(x)|$. The distance between two vertices x and y, denoted $d(x, y)$, is the length of a shortest x–y path in G. For any two edges $e_1 = xy$ and $e_2 = uv$ of G, define $d(x, e_2) = \min\{d(x, u), d(x, v)\}$ and the distance between edges as $D(e_1, e_2) = \min\{d(x, e_2), d(y, e_2)\} = \min\{d(u, e_1), d(v, e_1)\}$. The eccentricity, $\varepsilon(v)$ of a vertex $v \in V$ is the maximum distance between v and any other vertex in G.

For an edge $e_1 = xy$, the values $n_x(e_1)$ and $m_x(e_1)$ are defined to be the number of vertices and edges of G respectively whose distance to the vertex x is smaller than the distance to the vertex y. Similarly, $n_y(e_1)$ and $m_y(e_1)$ are defined to be the number of vertices and edges of G respectively whose distance to the vertex y is smaller than the distance to the vertex x. Mathematically, $n_x(e_1) = |\{a \in V(G) : d(x, a) < d(y, a)\}|$, $n_y(e_1) = |\{a \in V(G) : d(y, a) < d(x, a)\}|$, $m_x(e_1) = |\{e_2 \in E(G) : d(x, e_2) < d(y, e_2)\}|$, $m_y(e_1) = |\{e_2 \in E(G) : d(y, e_2) < d(x, e_2)\}|$.

A common matrix associated with a graph G is the adjacency matrix $A = (a_{ij})$, where

$$a_{ij} = \begin{cases} 1 & \text{if vertices } i \text{ and } j \text{ are adjacent,} \\ 0 & \text{otherwise.} \end{cases}$$

The characteristic polynomial of G is $p_G(\lambda) = \det(\lambda I - A)$, and its eigenvalues are the roots of this polynomial. The multiset of these eigenvalues forms the spectrum of G. The information that connects a graph with the spectrum of the matrix is provided by spectral graph theory [3,5].

The *energy* of a graph G of order p with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_p$ is defined as

$$E(G) = \sum_{i=1}^{p} |\lambda_i|.$$

The fundamental properties of a graph are closely tied to its eigenvalues, which play a crucial role in various mathematical and chemical analyzes. Among these, graph energy stands out as one of the earliest and most significant indices. A remarkable application of spectral graph theory in chemistry arises from the strong correlation between a graph's eigenvalues and the molecular orbital energy levels of π-electrons in conjugated hydrocarbons. This connection has been widely studied and applied in theoretical chemistry. In 1978 [12], I. Gutman extended the concept to arbitrary graphs, introducing a novel spectral invariant known as graph energy.

The *closeness matrix* $C(G) = (c_{uv})$ of order p is defined [30,31] by

$$c_{uv} = \begin{cases} 2^{-d(u,v)} & \text{if } u \neq v, \\ 0 & \text{if } u = v. \end{cases}$$

Its eigenvalues, denoted by $\alpha_1, \alpha_2, \ldots, \alpha_p$, form the *closeness spectrum* $CSpec(G)$. Their multiplicities m_i are typically arranged as:

$$CSpec(G) = \begin{pmatrix} \alpha_1 & \alpha_2 & \cdots & \alpha_p \\ m_1 & m_2 & \cdots & m_p \end{pmatrix}.$$

The *closeness energy* is then given by:

$$CE(G) = \sum_{i=1}^{p} |\alpha_i|.$$

The closeness matrix provides a robust quantitative framework for representing molecular structures. It enables the analysis of various structural attributes such as stability, reactivity, and physicochemical properties of chemical compounds. As a result, it has become an essential tool in computational chemistry and cheminformatics, offering valuable insights through spectral analysis.

Research on closeness energy opens promising avenues in mathematical chemistry, nanotechnology, drug discovery, and theoretical graph theory. By enhancing our understanding of molecular connectivity and spectral characteristics, closeness energy contributes both to fundamental scientific exploration and to practical applications in material science and pharmaceutical development.

Table 1: Benzenoid hydrocarbon compounds (BHC) with molecular names and structures

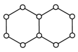
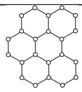
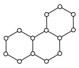
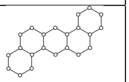
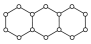
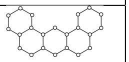
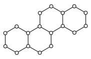
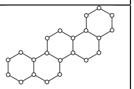
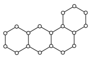
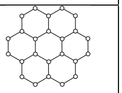
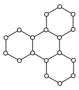
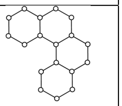
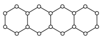
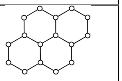
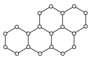
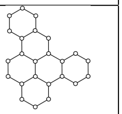
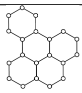
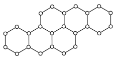
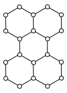
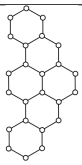
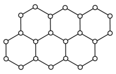
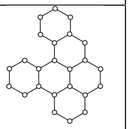
BHC	Molecular Name	Structure	BHC	Molecular Name	Structure
G_1	Naphthalene		G_{12}	Benzo[ghi]perylene	
G_2	Phenanthrene		G_{13}	Dibenz[a,h]anthracene	
G_3	Anthracene		G_{14}	Dibenz[a,j]anthracene	
G_4	Chrysene		G_{15}	Picene	
G_5	Tetraphene		G_{16}	Coronene	
G_6	Triphenylene		G_{17}	Benzo[c]phenanthrene	
G_7	Naphthacene		G_{18}	Pyrene	
G_8	Benzo[a]pyrene		G_{19}	Dibenzo[a,e]pyrene	
G_9	Benzo[e]pyrene		G_{20}	Dibenzo[a,h]pyrene	
G_{10}	Perylene		G_{21}	Dibenzo[a,i]pyrene	
G_{11}	Anthanthrene		G_{22}	Dibenzo[a,l]pyrene	

Table 2: Topological indices and their corresponding mathematical expressions

Topological Index	**Mathematical Expression**
Wiener [28]	$W(G) = \sum\limits_{u,v \in V(G)} d(u,v)$
Szeged [13]	$Sz(G) = \sum\limits_{e=uv \in E(G)} n_u(e) \cdot n_v(e)$
PI [22]	$PI(G) = \sum\limits_{e=uv \in E(G)} (n_u(e) + n_v(e))$
Revised Szeged [23]	$Sz^*(G) = \sum\limits_{e=uv \in E(G)} m_u(e) \cdot m_v(e)$
Eccentricity Connectivity [26]	$\xi^c(G) = \sum\limits_{v \in V(G)} d(v) \cdot \varepsilon(v)$
Total Eccentricity [8]	$\zeta(G) = \sum\limits_{v \in V(G)} \varepsilon(v)$
Second ABC [11]	$ABC_2(G) = \sum\limits_{e=uv \in E(G)} \sqrt{\frac{d_u+d_v-2}{d_u d_v}}$
Second GA [7]	$GA_2(G) = \sum\limits_{e=uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u+d_v}$
Fifth ABC [9]	$ABC_5(G) = \sum\limits_{e=uv \in E(G)} \sqrt{\frac{(d_u-1)(d_v-1)}{d_u+d_v-2}}$
Fourth GA [10]	$GA_4(G) = \sum\limits_{e=uv \in E(G)} \frac{2\sqrt{(d_u-1)(d_v-1)}}{d_u+d_v-2}$
Schultz [25]	$S(G) = \sum\limits_{e=uv \in E(G)} (d_u + d_v) \cdot d_{uv}$
Degree Distance [6]	$DD(G) = \sum\limits_{v \in V(G)} d_G(v) D(v)$
Gutman [14]	$Gut(G) = \sum\limits_{e=uv \in E(G)} d_u d_v D_{uv}$
Additive Harary [1]	$H_A(G) = \sum\limits_{u,v \in V(G)} \frac{d_u+d_v}{d(u,v)}$
Multiplicative Harary [29]	$H_M(G) = \sum\limits_{u,v \in V(G)} \frac{d_u d_v}{d(u,v)}$

2. Methodology

We first constructed the adjacency matrix for the molecular graphs of benzenoid hydrocarbons. From these matrices, we determined the characteristic polynomials and computed the corresponding eigenvalues. Similarly, we derived the closeness matrix and obtain the closeness eigenvalues for these molecular structures. The experimental physicochemical properties of the studied hydrocarbons (such as boiling point and enthalpy of formation, and related properties) were taken from previously published studies [21,2], and these values were used for correlation and regression analyses. All eigenvalue computations were performed using MATLAB software. Additionally, we investigated the edge connectivity of benzenoid hydrocarbons by considering the degrees of the end vertices of each edge. Using edge partitioning techniques, we computed various distance-based and degree-based topological indices for these molecular graphs. To examine the relationships among these indices, we conducted correlation analysis using SPSS software.

3. Results and Discussions

3.1. Significance of energy $E(G)$ and closeness energy $CE(G)$

Table 3: Energy $E(G)$ and closeness energy $CE(G)$ of various benzenoid hydrocarbons

BHC	$E(G)$	$CE(G)$	**BHC**	$E(G)$	$CE(G)$
Naphthalene	13.6832	10.0000	Benzo[ghi]perylene	31.4251	15.4110
Phenanthrene	19.4483	9.5928	Dibenz[a,h]anthracene	30.8805	15.2784
Anthracene	19.3137	9.4583	Dibenz[a,j]anthracene	30.8795	15.2571
Chrysene	25.1922	12.3993	Picene	30.9432	15.2470
Tetraphene	25.1040	12.3920	Coronene	34.5718	16.9156
Triphenylene	25.2760	12.3946	Benzo[c]phenanthrene	13.2523	12.4051
Naphthacene	25.3179	12.4082	Pyrene	22.5055	11.0609
Benzo[a]pyrene	28.2220	13.8588	Dibenzo[a,e]pyrene	34.6040	16.7460
Benzo[e]pyrene	28.3361	13.9083	Dibenzo[a,h]pyrene	33.9278	16.7454
Perylene	28.2453	13.6876	Dibenzo[a,i]pyrene	34.0180	16.6918
Anthanthrene	31.2529	15.5131	Dibenzo[a,l]pyrene	34.0304	16.6567

In this section, we have evaluated the predictive potential of certain physicochemical properties of polycyclic aromatic hydrocarbons by analyzing the graph energy and closeness energy derived from a dataset consisting of 22 benzenoid hydrocarbons, whose molecular structures are shown in Table 1. The dataset was sourced from [2]. Based on their standard definitions, we have calculated both energy and closeness energy for each benzenoid hydrocarbon discussed in this study. The results for energy and closeness energy are presented in Table 3. Table 4 provides the experimental data for various physicochemical characteristics of the molecules.

Additionally, by employing edge partitioning, we computed several well-established distance-based and degree-based topological indices (listed in Table 2) according to their respective formal definitions. The computed topological indices for the benzenoid hydrocarbons are presented in Table 5 and Table 6. The correlation coefficients (r) between graph energy and closeness energy and the molecular properties, like boiling point (BP), solubility (S), logarithm of the partition coefficient (log P), and enthalpy of formation ΔH_f are summarized in Table 7.

To further investigate these relationships, we utilized the following linear regression model:

$$Y = b(\pm 2e) + m(\pm 2e)X \tag{3.1}$$

In this model, Y denotes the molecular property, X represents the topological index, e is the standard error of the coefficients, b is the intercept, and m is the slope. Using Equation 3.1, we developed linear regression models in the subsequent subsections for predicting BP, S, log P, and ΔH_f based on both energy and closeness energy. Moreover, we analyzed the correlation between these energy-based indices

Table 4: Benzenoid hydrocarbon compounds (BHC) with physico-chemical properties

BHC	BP	S	$\log P$	ΔH_f
Naphthalene	218	79.38	3.3	150.6
Phenanthrene	338	93.79	4.46	209.1
Anthracene	340.05	92.43	4.45	218.3
Chrysene	431	106.83	5.81	267.7
Tetraphene	425	108.22	5.76	276.9
Triphenylene	429	104.66	5.49	258.5
Naphthacene	440	105.47	5.76	286.1
Benzo[a]pyrene	496	111.85	6.13	279.9
Benzo[e]pyrene	493	110.46	6.44	289.1
Perylene	497	109.10	6.25	279.9
Anthanthrene	547	114.10	7.04	310.5
Benzo[ghi]perylene	542	114.10	6.63	301.3
Dibenz[a,h]anthracene	536	119.87	6.75	335.5
Dibenz[a,j]anthracene	531	119.87	6.54	335.5
Picene	519	119.87	7.11	326.3
Coronene	590	116.36	7.64	322.7
Benzo[c]phenanthrene	448	113.61	5.70	280.5
Pyrene	404	96.06	4.88	230.5
Dibenzo[a,e]pyrene	592	124.89	7.28	338.5
Dibenzo[a,h]pyrene	596	123.50	7.28	347.7
Dibenzo[a,i]pyrene	594	123.50	7.28	347.7
Dibenzo[a,l]pyrene	595	131.69	7.71	351.2

Table 5: Topological indices (Set 1) for 22 benzenoid hydrocarbon compounds: includes the first eight indices.

Graph G	W	Sz	PI	Sz^*	ξ^c	ζ	ABC_2	GA_2
Naphthalene	109	243	110	243	90	42	6.6348	10.3321
Phenanthrene	271	632	224	632	170	76	8.9123	14.3151
Anthracene	279	656	224	656	180	80	8.7832	14.5652
Chrysene	545	1301	378	1301	280	122	10.9038	18.2377
Tetraphene	553	1325	378	1325	284	124	10.8171	18.4002
Triphenylene	513	1269	378	1269	246	108	11.1554	17.9443
Naphthacene	569	1381	378	1381	298	130	10.6392	18.7628
Benzo[a]pyrene	680	1887	480	1887	318	135	11.7507	21.1290
Benzo[e]pyrene	652	1852	480	1852	286	122	11.9476	20.8792
Perylene	654	1858	480	1858	286	122	11.9347	20.9093
Anthanthrene	839	2613	594	2613	356	148	12.5264	23.9991
Benzo[ghi]perylene	815	2571	594	2571	326	136	12.6759	23.7700
Dibenz[a,h]anthracene	971	2354	572	2354	424	182	12.6474	22.2458
Dibenz[a,j]anthracene	955	2290	572	2290	402	173	12.7669	21.9720
Picene	963	2330	572	2330	424	182	12.6888	22.1458
Coronene	1002	3438	720	3438	366	150	13.3525	26.6202
Benzo[c]phenanthrene	529	1253	378	1253	257	113	11.0589	17.9251
Pyrene	362	1008	304	1008	200	86	9.8540	17.2468
Dibenzo[a,e]pyrene	1082	3095	696	3095	411	174	13.7897	24.6088
Dibenzo[a,h]pyrene	1142	3174	696	3174	466	196	13.4819	25.0097
Dibenzo[a,i]pyrene	1142	3174	696	3174	466	196	13.4819	25.0097
Dibenzo[a,l]pyrene	1066	3023	696	3023	392	166	13.9063	24.3438

Table 6: Topological indices (Set 2) for the same 22 benzenoid hydrocarbon compounds: includes the remaining seven indices.

BHC	ABC_5	GA_4	S	DD	Gut	H_A	H_M
Naphthalene	6.7465	10.9342	520	470	505	106.9333	119.2667
Phenanthrene	8.9138	15.9468	1284	1208	1342	192.1381	224.0381
Anthracene	8.7255	15.9468	1324	1248	1392	189.9429	220.4095
Chrysene	10.7115	20.9498	2584	2482	2819	289.6683	345.1540
Tetraphene	10.6407	20.9498	2624	2522	2869	287.4730	341.5254
Triphenylene	11.2357	20.9574	2424	2322	2619	295.6143	354.3143
Naphthacene	10.4353	20.9558	2704	2602	2969	284.3079	336.5127
Benzo[a]pyrene	12.2659	23.9427	3302	3182	3712	361.6492	443.5611
Benzo[e]pyrene	12.7541	23.9515	3160	3040	3532	366.8238	451.6238
Perylene	12.7541	23.9515	3172	3052	3550	366.4286	450.9286
Anthanthrene	13.8203	26.9356	4156	4018	4797	437.9683	548.9730
Benzo[ghi]perylene	14.2725	26.9455	4032	3894	4637	442.3714	555.9381
Dibenz[a,h]anthracene	12.1914	25.9529	4620	4492	5186	394.3676	474.8446
Dibenz[a,j]anthracene	12.4469	25.9412	4540	4412	5086	395.6405	476.6024
Picene	12.1914	25.9529	4580	4452	5136	396.5628	478.4732
Coronene	15.7909	29.9396	5040	4884	5934	522.2571	667.2571
Benzo[c]phenanthrene	11.0825	20.9240	2504	2402	2719	292.0286	348.6119
Pyrene	10.6109	18.9468	1770	1676	1933	255.4048	309.7048
Dibenzo[a,e]pyrene	14.3924	28.9390	5228	5082	5951	485.3937	601.8246
Dibenzo[a,h]pyrene	13.6777	28.9469	5530	5384	6331	477.2581	589.6208
Dibenzo[a,i]pyrene	13.6760	28.9529	5530	5384	6331	477.2581	589.6208
Dibenzo[a,l]pyrene	14.6771	28.9324	5148	5002	5851	487.7540	605.2825

Table 7: Correlation between energy $E(G)$, closeness energy $CE(G)$, and molecular properties of benzenoid hydrocarbon compounds

	BP	S	$\log P$	ΔH_f
Energy	0.9040	0.8157	0.9031	0.8615
Closeness Energy	0.9572	0.9166	0.9602	0.9285

and various distance and degree based topological indices previously introduced in the paper, with the results shown in Table 8.

Linear regression was selected for this study due to its interpretability, simplicity, and frequent use in quantitative structure-property relationship (QSPR) analyses. Given the relatively small dataset of 22 benzenoid hydrocarbons, linear models provide a reliable first-level approach to identify direct associations between graph-based indices and physicochemical properties while minimizing the risk of overfitting that can arise from more complex models. This choice ensures both clarity in interpretation and comparability with prior studies in chemical graph theory.

The regression models yielded strong R^2 values, showing that energy and closeness energy are effective descriptors for predicting physicochemical properties of benzenoid hydrocarbons. The correlation coefficients (r) supported this observation, while the standard error values confirmed the predictive accuracy of the models.

Table 8: Correlation between topological indices and energy $E(G)$ and closeness energy $CE(G)$ for benzenoid hydrocarbon compounds

TIs	**Energy**	**Closeness Energy**
W	0.949	0.975
Sz	0.954	0.983
PI	0.965	0.987
Sz^*	0.954	0.983
ξ^c	0.922	0.925
ζ	0.906	0.908
ABC_2	0.947	0.952
GA_2	0.967	0.964
ABC_5	0.733	0.711
GA_4	0.967	0.972
S	0.955	0.981
DD	0.954	0.980
Gut	0.957	0.984
H_A	0.960	0.977
H_M	0.955	0.973

3.2. The linear regression models with respect to energy $E(G)$

In this subsection we have derived the linear regression models for BP, S, log P and ΔHf using the least square fitting procedure with the help of energy of graph ($E(G)$) and the data given in Table 3 and Table 4, respectively. Throughout the paper the symbols N, S_e and F stand for population, standard error of the estimates and F-values respectively.

$$\begin{aligned} \mathrm{BP} &= 99.819\,(\pm 42.604) + 13.964\,(\pm 1.518)\,E(G) \\ N &= 22, \quad S_e = 44.31607, \quad F = 84.57199 \end{aligned}$$

$$\begin{aligned} \mathrm{S} &= 68.008\,(\pm 7.116) + 1.567\,(\pm 0.253)\,E(G) \\ N &= 22, \quad S_e = 7.402889, \quad F = 38.18548 \end{aligned}$$

$$\begin{aligned} \log P &= 1.737\,(\pm 0.491) + 0.161\,(\pm 0.017)\,E(G) \\ N &= 22, \quad S_e = 0.511722, \quad F = 85.2764 \end{aligned}$$

$$\begin{aligned} \Delta H_f &= 96.287\,(\pm 25.814) + 7.02\,(\pm 0.92)\,E(G) \\ N &= 22, \quad S_e = 26.85173, \quad F = 58.2265 \end{aligned}$$

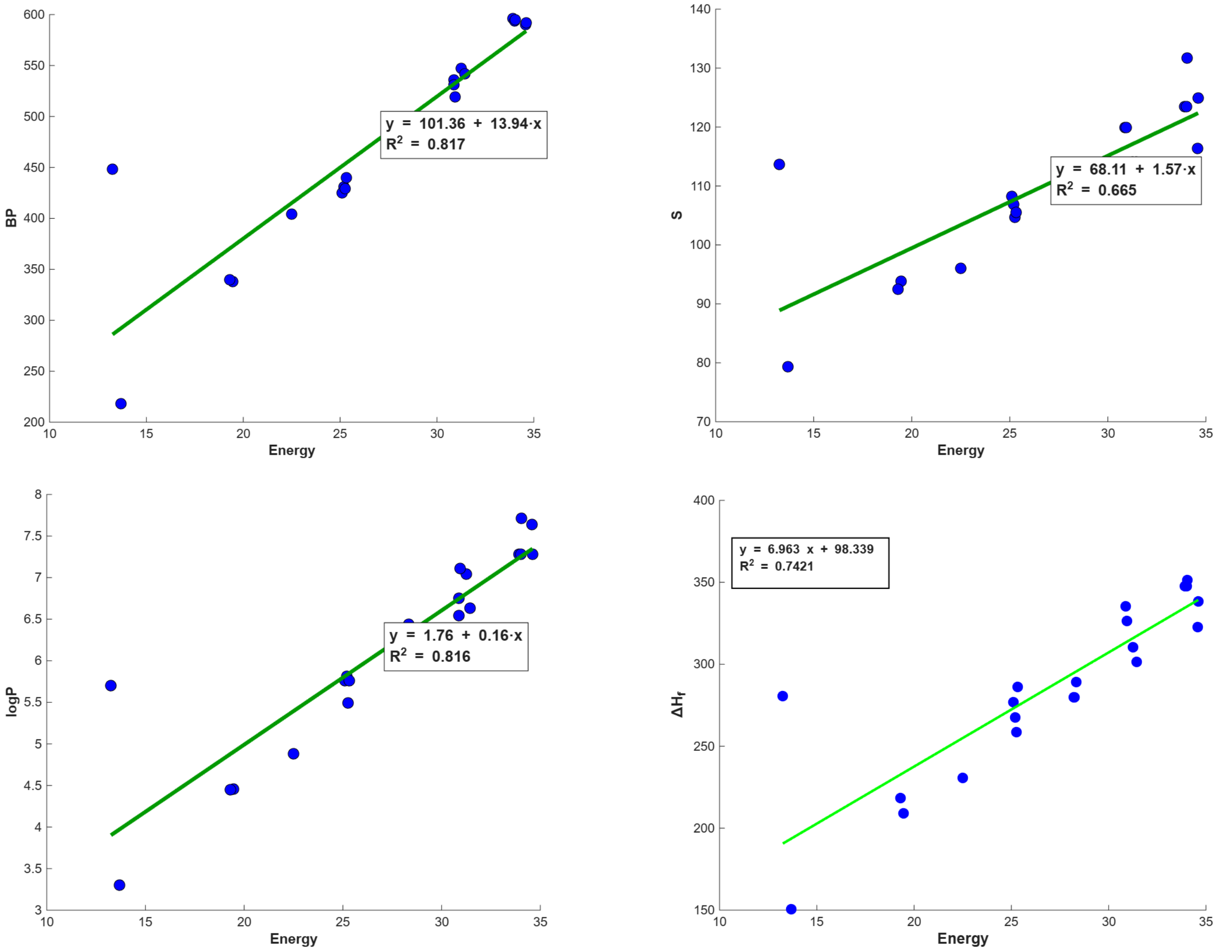


Figure 1: Scatter plots showing the correlation of boiling point (BP), entropy (S), logarithm of partition coefficient (log P), and enthalpy of formation (ΔH_f) with energy $E(G)$ for 22 benzenoid hydrocarbons. (a)–(d) correspond to the respective properties.

$$\begin{aligned}
W &= 630\,(\pm 102.0292) + 48.98\,(\pm 3.644)\,E(G)\\
N &= 22, \quad S_e = 98.693, \quad F = 180.685
\end{aligned}$$

$$\begin{aligned}
Sz &= 2180\,(\pm 296.929) + 152\,(\pm 10.599)\,E(G)\\
N &= 22, \quad S_e = 287.043, \quad F = 201.376
\end{aligned}$$

$$\begin{aligned}
PI &= 303\,(\pm 49.039) + 28.64\,(\pm 1.750)\,E(G)\\
N &= 22, \quad S_e = 47.406, \quad F = 267.672
\end{aligned}$$

$$\begin{aligned}
Sz^* &= 2180\,(\pm 296.929) + 152\,(\pm 10.599)\,E(G)\\
N &= 22, \quad S_e = 287.043, \quad F = 201.376
\end{aligned}$$

$$\begin{aligned}
EC &= 115\,(\pm 41.150) + 15.68\,(\pm 1.469)\,E(G)\\
N &= 22, \quad S_e = 39.780, \quad F = 113.889
\end{aligned}$$

$$\begin{aligned}
TE &= 38.43\,(\pm 18.436) + 6.31\,(\pm 0.068)\,E(G)\\
N &= 22, \quad S_e = 17.822, \quad F = 92.085
\end{aligned}$$

$$\begin{aligned}
ABC_2 &= 3.52\,(\pm 0.631) + 0.3\,(\pm 0.023)\,E(G)\\
N &= 22, \quad S_e = 0.6096374, \quad F = 172.497
\end{aligned}$$

$$\begin{aligned}
GA_2 &= 2.04\,(\pm 1.105) + 0.67\,(\pm 0.039)\,E(G)\\
N &= 22, \quad S_e = 1.0682689, \quad F = 290.628
\end{aligned}$$

$$\begin{aligned}
ABC_5 &= 3.69\,(\pm 1.8338) + 0.32\,(\pm 0.066)\,E(G)\\
N &= 22, \quad S_e = 1.7768531, \quad F = 23.193
\end{aligned}$$

$$\begin{aligned}
GA_5 &= 0.96\,(\pm 1.353) + 0.82\,(\pm 0.048)\,E(G)\\
N &= 22, \quad S_e = 1.3078435, \quad F = 288.388
\end{aligned}$$

$$\begin{aligned}
S &= 3150\,(\pm 470.498) + 241\,(\pm 16.795)\,E(G)\\
N &= 22, \quad S_e = 454.833, \quad F = 205.424
\end{aligned}$$

$$\begin{aligned}
DD &= 3150\,(\pm 466.568) + 236\,(\pm 16.654)\,E(G)\\
N &= 22, \quad S_e = 451.034, \quad F = 201.227
\end{aligned}$$

$$\begin{aligned}
GU &= 3910\,(\pm 540.018) + 284\,(\pm 19.276)\,E(G)\\
N &= 22, \quad S_e = 522.038, \quad F = 216.842
\end{aligned}$$

$$\begin{aligned}
H_A &= 140\,(\pm 32.831) + 18.04\,(\pm 1.172)\,E(G)\\
N &= 22, \quad S_e = 31.7374801, \quad F = 236.930
\end{aligned}$$

$$\begin{aligned}
H_M &= 207\,(\pm 45.490) + 23.34\,(\pm 1.624)\,E(G)\\
N &= 22, \quad S_e = 43.9752678, \quad F = 206.689
\end{aligned}$$

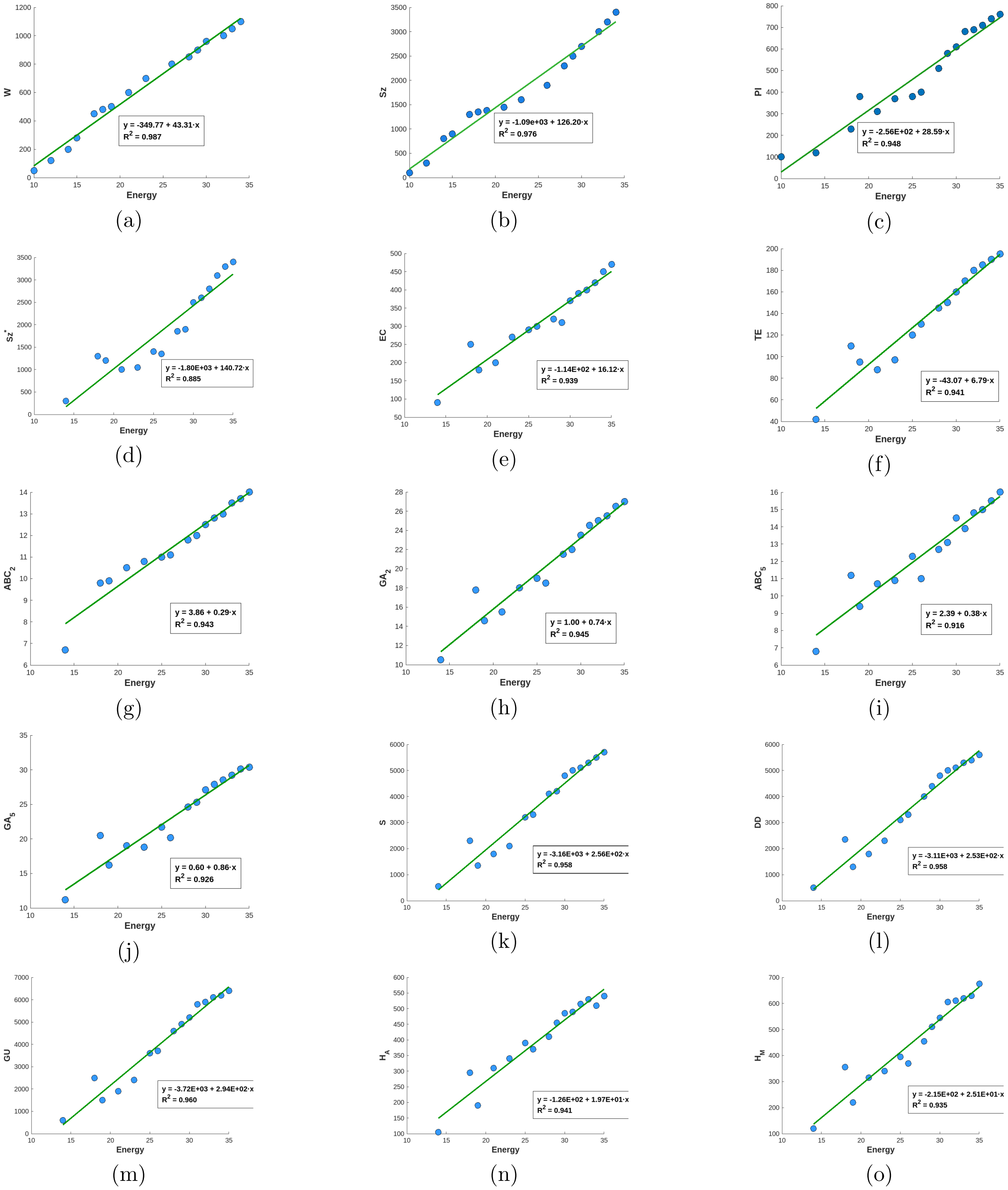


Figure 2: Scatter plots showing the correlation of selected topological indices (as listed in Table 2) with energy $E(G)$ for 22 benzenoid hydrocarbons.

3.3. The linear regression models with respect to closeness energy $CE(G)$

$$\begin{aligned} \text{BP} &= -56.84\,(\pm 36.947) + 38.98\,(\pm 2.635)\,CE(G) \\ N &= 22, \quad S_e = 29.322, \quad F = 218.858 \end{aligned}$$

$$\begin{aligned} \text{S} &= 46.617\,(\pm 6.361) + 4.651\,(\pm 0.453)\,CE(G) \\ N &= 22, \quad S_e = 5.049, \quad F = 105.079 \end{aligned}$$

$$\begin{aligned} \log P &= -0.092\,(\pm 0.413) + 0.453\,(\pm 0.029)\,CE(G) \\ N &= 22, \quad S_e = 0.328, \quad F = 236.205 \end{aligned}$$

$$\begin{aligned} \Delta H_f &= 14.508\,(\pm 24.841) + 19.817\,(\pm 1.771)\,CE(G) \\ N &= 22, \quad S_e = 19.714, \quad F = 125.112 \end{aligned}$$

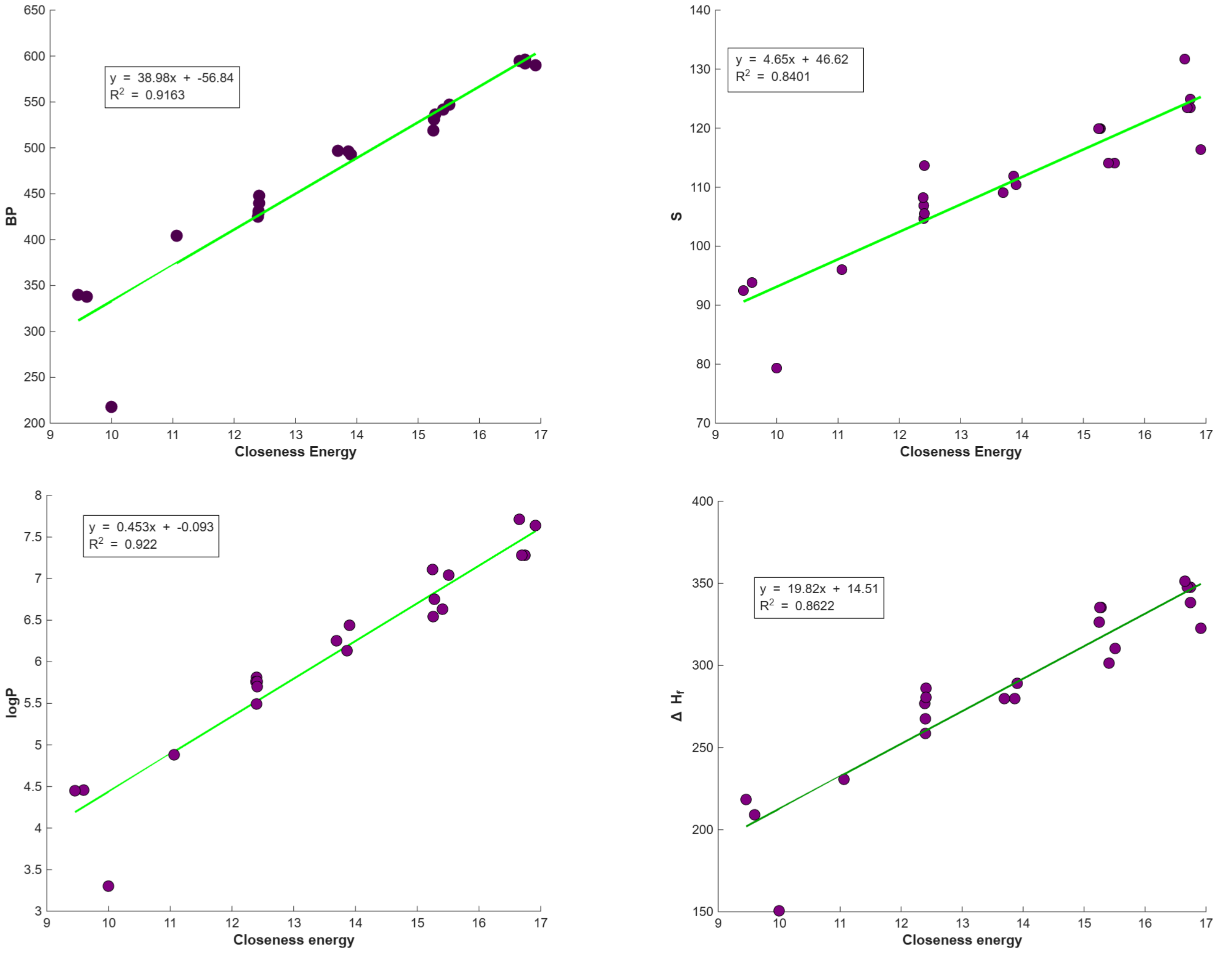


Figure 3: Scatter plots showing the correlation of boiling point (BP), entropy (S), logarithm of partition coefficient (log P), and enthalpy of formation (ΔH_f) with closeness energy $CE(G)$ for 22 benzenoid hydrocarbons. (a)–(d) correspond respectively to BP, S, log P, and ΔH_f.

$$W = 980\,(\pm 87.090) + 123\,(\pm 6.211)\,CE(G)$$
$$N = 22, \quad S_e = 69.117, \quad F = 389.180$$

$$Sz = 3270\,(\pm 218.215) + 377\,(\pm 15.563)\,CE(G)$$
$$N = 22, \quad S_e = 173.182, \quad F = 588.156$$

$$PI = 504\,(\pm 35.973) + 71.34\,(\pm 2.566)\,CE(G)$$
$$N = 22, \quad S_e = 28.549, \quad F = 773.210$$

$$Sz^* = 3270\,(\pm 218.215) + 377\,(\pm 15.563)\,CE(G)$$
$$N = 22, \quad S_e = 173.182, \quad F = 588.156$$

$$EC = 214\,(\pm 49.315) + 38.26\,(\pm 3.517)\,CE(G)$$
$$N = 22, \quad S_e = 39.138, \quad F = 118.319$$

$$TE = 78.15\,(\pm 22.238) + 15.4\,(\pm 1.586)\,CE(G)$$
$$N = 22, \quad S_e = 17.649, \quad F = 94.291$$

$$ABC_2 = 1.62\,(\pm 0.729) + 0.72\,(\pm 0.052)\,CE(G)$$
$$N = 22, \quad S_e = 0.5787012, \quad F = 193.628$$

$$GA_2 = 2.07\,(\pm 1.412) + 1.63\,(\pm 0.101)\,CE(G)$$
$$N = 22, \quad S_e = 1.1208625, \quad F = 262.161$$

$$ABC_5 = 2.04\,(\pm 2.312) + 0.75\,(\pm 0.165)\,CE(G)$$
$$N = 22, \quad S_e = 1.8352596, \quad F = 20.488$$

$$GA_5 = 4.26\,(\pm 1.533) + 2.01\,(\pm 0.109)\,CE(G)$$
$$N = 22, \quad S_e = 1.2169822, \quad F = 336.156$$

$$S = 4870\,(\pm 375.342) + 602\,(\pm 26.769)\,CE(G)$$
$$N = 22, \quad S_e = 297.884, \quad F = 505.546$$

$$DD = 4840\,(\pm 373.358) + 591\,(\pm 26.627)\,CE(G)$$
$$N = 22, \quad S_e = 296.308, \quad F = 492.586$$

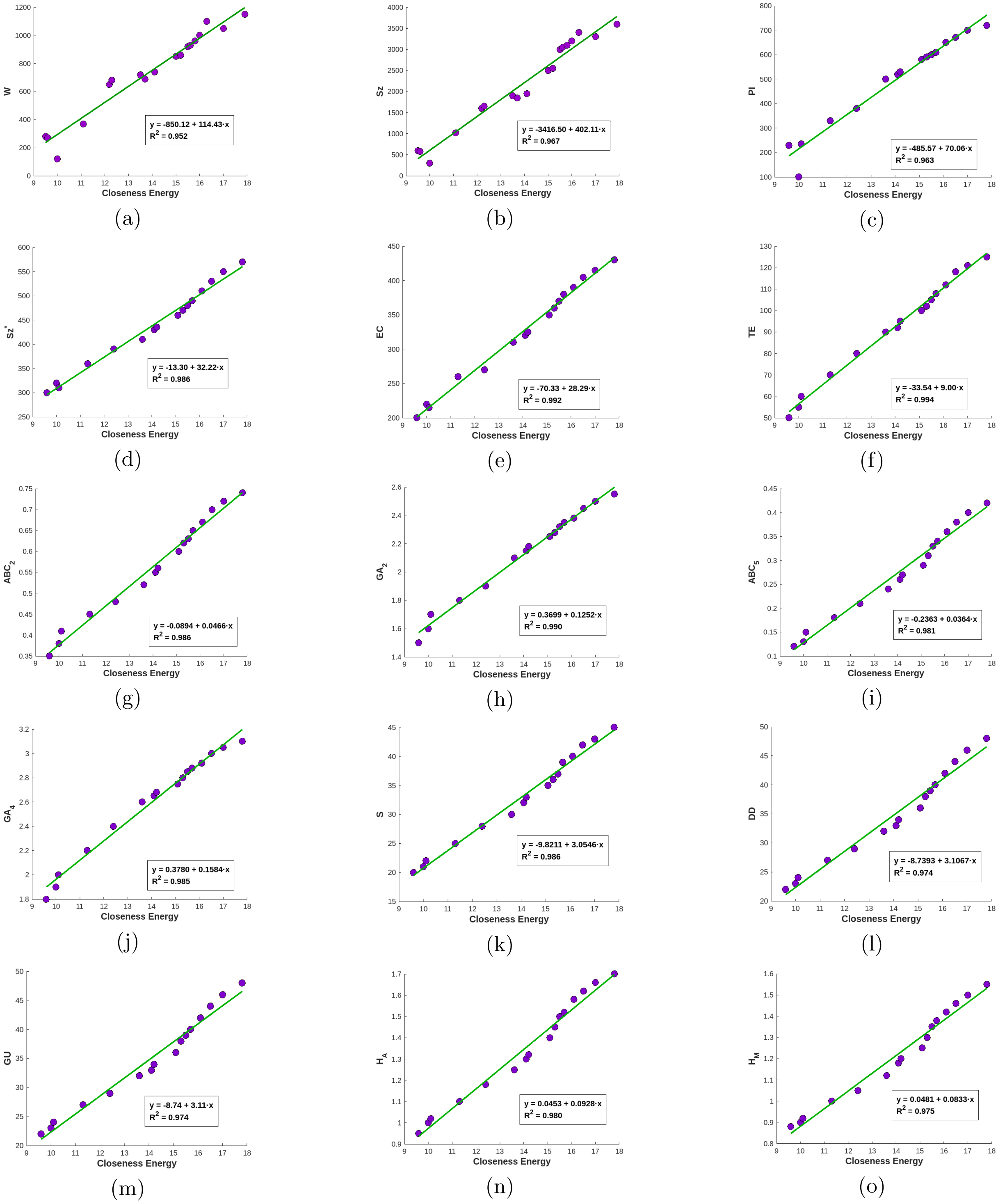
$$GU = 5940\,(\pm 408.571) + 71\,(\pm 29.139)\,CE(G)$$
$$N = 22, \quad S_e = 324.255, \quad F = 593.890$$

$$H_A = 263\,(\pm 30.359) + 44.68\,(\pm 2.165)\,CE(G)$$
$$N = 22, \quad S_e = 24.0938659, \quad F = 425.806$$

$$H_M = 367\,(\pm 43.105) + 57.89\,(\pm 3.074)\,CE(G)$$
$$N = 22, \quad S_e = 34.2098698, \quad F = 354.480$$

A scatter plot utilizes dots to represent values for two distinct numerical variables, allowing for the visualization of potential relationships between them. In this study, scatter plots were employed to examine the correlation of boiling point (BP), entropy (S), logarithm of partition coefficient (log P), and enthalpy of formation (ΔH_f) of benzenoid hydrocarbons with energy and closeness energy. Figure 1 and Figure 3 display the scatter plots of BP, S, lop P, and ΔH_f in relation to energy $E(G)$ and closeness energy $CE(G)$, respectively. Additionally, Figure 2 and Figure 4 present the scatter plots of various topological indices, listed in Table 2 with respect to $E(G)$ and $CE(G)$, respectively.

Our findings are consistent with earlier studies on benzenoid hydrocarbons that analyzed graph energy $E(G)$ and related eigenvalue-based measures, which were shown to correlate well with physicochemical



(a) (b) (c)

(d) (e) (f)

(g) (h) (i)

(j) (k) (l)

(m) (n) (o)

Figure 4: Scatter plots showing the correlation of selected topological indices (as listed in Table 2) with closeness energy $CE(G)$ for 22 benzenoid hydrocarbons.

properties such as boiling point, solubility, log P, and enthalpy of formation [2,21]. In this study, by investigating the closeness energy $CE(G)$ for the same set of 22 compounds, we observed stronger correlations with these properties (Table 7). This indicates that closeness energy captures molecular connectivity more effectively than graph energy alone. In addition, we found strong linear relationships between $CE(G)$ and well-known distance-based indices such as Wiener, Szeged, and PI (Table 7 and Table 8), further supporting its role as a useful descriptor. Taken together, this shows that closeness energy not only complements graph energy but also provides improved predictive power for structure–property modeling of benzenoid hydrocarbons.

4. Conclusion

This study systematically evaluated the energy, closeness energy, and a suite of distance, degree, and eccentricity-based topological indices for 22 benzenoid hydrocarbons. The results confirmed that these indices capture structural variation and exhibit meaningful correlations with physicochemical properties such as boiling point, solubility, hydrophobicity, and enthalpy of formation. In particular, closeness energy emerged as a complementary descriptor that strengthens predictive modeling compared to classical graph energy alone.

By combining analytical derivations, computational evaluations, and regression analysis, the study demonstrates that topological descriptors provide valuable insight into molecular connectivity and property trends. While the linear models yielded strong coefficients of determination for several properties, the predictive scope is limited by dataset size and the inherent dependence of indices on molecular size.

Future work will extend this framework to larger datasets, include isomeric comparisons to improve scaling, and explore nonlinear and machine learning methods for enhancing predictive accuracy. Beyond chemical graph theory, the findings underscore the versatility of graph-based descriptors and their potential applications across cheminformatics, materials science, and computational modeling.

Acknowledgement

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Availability of data and software

The experimental data for benzenoid hydrocarbons were obtained from reference [2,21]. Eigenvalues of the corresponding molecular graphs were computed using MATLAB, and statistical analyses were conducted using SPSS software.

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