

ON SOME EXTENDED ENERGY OF GRAPHS AND THEIR APPLICATIONS

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Abstract: In this paper, we established a relation between the extended energy of graphs such as the first and second Zagreb energy, Randić energy, reciprocal Randić energy, and the atom-bond connectivity energy with some thermodynamic properties of benzenoid hydrocarbons. We have seen that these indices are well correlated to the boiling point (BP), Kovats retention index (RI), entropy (S), enthalpy of formation (ΔH_f), octanol-water partition coefficient ($\log P$), and acentric factor (ω) of benzenoid hydrocarbons.

Keywords: Degree-based topological index, extended adjacency matrix, extended energy.

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1. INTRODUCTION

Graph theory, play an important role in various fields like Chemistry, Computer Science, Operations Research and also in real life. Graphs are used to model many real world problems. In Mathematical Chemistry, a molecular graph is a representation of the molecule in terms of graph whose vertices correspond to the atoms and bonds between them are considered as edges. We refer the reader to [1, 2, 3, 4, 5, 6], for some recent studies and applications of graphs in some different fields. In this paper, all graphs are assumed to be finite, simple, and connected. Let $G \cong (V, E)$ be a graph of order n and size m , with vertex set $V(G) = \{v_1, v_2, v_3, \dots, v_n\}$. If the two vertices v_i and v_j are connected by a line (adjacent), we denote it as $v_i v_j \in E(G)$. The elements of $E(G)$ are called edges of G . The degree of a vertex $v_i \in G$ is the number of adjacent vertices to v_i and it is denoted by d_i . A topological index (TI) or a molecular structure descriptor of a molecular graph is a real numeric quantity that characterizes the whole of its structural properties. Application of topological indices started in 1947 [7], when Harold Wiener introduced two parameters namely polarity number P or Wiener polarity index $W_P(G)$, which is the number of pairs of carbon atoms which are separated by three carbon-carbon bonds and the second parameter was path number W or Wiener index $W(G)$, which is the sum of the distance between any two carbon atoms in the molecule in terms of the carbon-carbon bond to predict the boiling points of different members of the alkane series. These two indices are defined as

$$W_P(G) = |\{(u, v) : d_G(u, v) = 3, u, v \in V(G)\}|$$

and

$$W(G) = \sum_{\{u, v\} \subseteq V} d_G(u, v)$$

where $d_G(u, v)$ or simply $d(u, v)$ is the distance between u and v in G . In recent days, researchers have introduced many kinds of topological indices such as degree-based topological indices, spectrum-based indices, etc. Topological indices are used to predict various physicochemical properties of organic molecules. It is an efficient method in avoiding expensive and time-consuming laboratory experiments. Topological indices play a significant role in QSPR and QSAR studies. QSPR/QSAR models are mathematical tools used to predict the biological and physicochemical properties of molecules. We refer the reader to [8, 9, 10, 11], for further study of topological indices and their applications. Generally, vertex degree-based topological indices are defined as

$$TI(G) = \sum_{v_i v_j \in E(G)} f(d_i, d_j).$$

Where, $f(x, y)$ denotes the function of x, y with the property $f(x, y) = f(y, x)$. Some well-known topological indices of these group are

- i. First Zagreb index [12], $f(d_i, d_j) = (d_i + d_j)$,
- ii. Second Zagreb index [12], $f(d_i, d_j) = d_i \cdot d_j$,
- iii. Randić index [13], $f(d_i, d_j) = \frac{1}{\sqrt{d_i \cdot d_j}}$,
- iv. Reciprocal Randić index [14], $f(d_i, d_j) = \sqrt{d_i \cdot d_j}$,
- v. Atom-bond connectivity index [15], $f(d_i, d_j) = \sqrt{\frac{d_i + d_j - 2}{d_i \cdot d_j}}$.

We refer the reader to [16, 17, 18, 19, 20, 21, 22, 23], for further study about these indices. Graph-theoretical matrices and derived molecular descriptors have played an important roles in QSPR and QSAR studies [24, 25, 26, 27, 28, 29, 30, 31]. There are many types of graph-theoretical matrices proposed in the literature, among the most important appear to be the adjacency matrix A . The adjacency matrix A of G is a square matrix of order n such that

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

The general extended matrix A_{TI} of G is a square matrix of order n such that

$$a_{i,j} = \begin{cases} f(d_i, d_j), & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0, & \text{otherwise.} \end{cases}$$

The extended energy of G is defined as

$$\mathcal{E}_{TI}(G) = \sum_{i=1}^n |\eta_i|,$$

where, $\eta_1, \eta_2, \dots, \eta_n$ are the eigenvalues of A_{TI} . There is an extended matrix associated with each of the Zagreb indices (first and second Zagreb index), Randić index, reciprocal Randić index, and atom-bond connectivity index. The first Zagreb matrix $Z^{(1)}$ and second Zagreb matrix $Z^{(2)}$ are defined as

$$Z^{(1)} = \begin{cases} d_i + d_j, & \text{if } v_i v_j \in E(G) \\ 0, & \text{otherwise,} \end{cases}$$

and

$$Z^{(2)} = \begin{cases} d_i d_j, & \text{if } v_i v_j \in E(G) \\ 0, & \text{otherwise.} \end{cases}$$

Suppose $\eta_1^{(1)}, \eta_2^{(1)}, \dots, \eta_n^{(1)}$ and $\eta_1^{(2)}, \eta_2^{(2)}, \dots, \eta_n^{(2)}$ are the eigenvalues of $Z^{(1)}$ and $Z^{(2)}$. The first Zagreb energy and second Zagreb energy [32], are defined as

$$ZE_1 = \sum_{i=1}^n |\eta_i^{(1)}|$$

and

$$ZE_2 = \sum_{i=1}^n |\eta_i^{(2)}|$$

respectively, $i = 1, 2, \dots, n$. The Randić matrix and reciprocal Randić matrix are defined as

$$(R)_{ij} = \begin{cases} \frac{1}{\sqrt{d_i d_j}}, & \text{if } v_i v_j \in E(G) \\ 0, & \text{otherwise,} \end{cases}$$

and

$$(RR)_{ij} = \begin{cases} \sqrt{d_i d_j}, & \text{if } v_i v_j \in E(G) \\ 0, & \text{otherwise.} \end{cases}$$

If the ζ'_i and ζ''_i , $i = 1, 2, \dots, n$ are the eigenvalues of $(R)_{ij}$ and $(RR)_{ij}$, then the Randić energy [33] and reciprocal Randić energy are defined as

$$RE = \sum_{i=1}^n |\zeta'_i|$$

and

$$RRE = \sum_{i=1}^n |\zeta''_i|.$$

The atom-bond connectivity matrix is defined as

$$(ABC)_{ij} = \begin{cases} \sqrt{\frac{d_i + d_j - 2}{d_i \cdot d_j}}, & \text{if } v_i v_j \in E(G) \\ 0, & \text{otherwise.} \end{cases}$$

If ξ_i , $i = 1, 2, \dots, n$ are the eigenvalues of $(ABC)_{ij}$, then the atom-bond connectivity energy [34], is defined as

$$ABCE = \sum_{i=1}^n |\xi_i|.$$

This study is directed toward assessing the predictive potential of the extended energy of graphs such as the first Zagreb energy, second Zagreb energy, Randić energy, reciprocal Randić energy, and the atom-bond connectivity energy. How they can help in chemical sciences or QSPR and QSAR studies. We studied their significance in predicting some thermodynamic properties of polycyclic aromatic compounds using a data set of 22-benzenoid hydrocarbons.

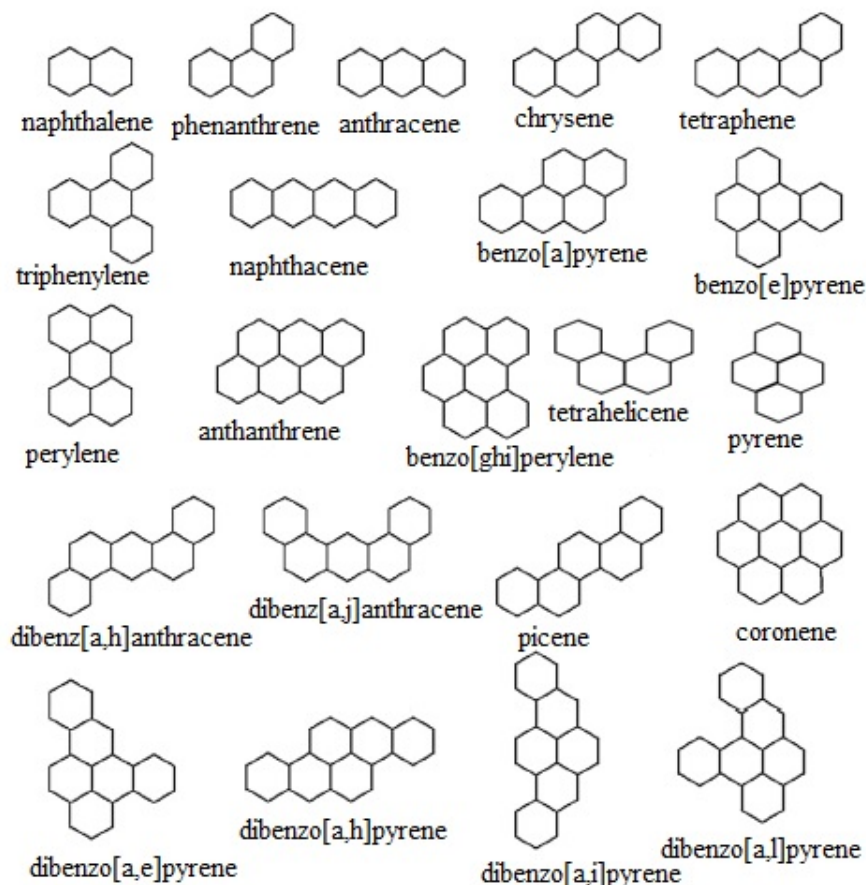


Figure 1: Molecular graphs of benzenoid hydrocarbons

2. METHODOLOGY

In the first step, we find out the extended adjacency matrix of the underlying molecular graphs according to the adjacency of the vertices. Then, using MATLAB software we found the eigenvalues of the corresponding molecular graphs. We used Microsoft Excel data analysis tools for the linear regression analysis.

3. RESULTS

3.1. Significance of extended energy

Based on a data set of 22-benzenoid hydrocarbons in this section, we studied the relationship between the first Zagreb energy (ZE_1), second Zagreb energy

Table 1: Energies of benzenoid hydrocarbons

Molecules \ Energies	ZE_1	ZE_2	RE	RRE	$ABCE$
naphthalene	61.2721742	68.97693444	6.26365546	30.41279872	9.63418932
phenanthrene	90.71477714	106.9667312	8.60006	45.02192128	13.62821686
anthracene	90.33884824	105.7300133	8.50104758	44.71465836	13.57960148
chrysene	120.069636	144.8831508	10.92607293	59.59086852	17.60537674
tetraphene	119.8665308	143.7999336	10.85023974	59.36535276	17.59025286
triphenylene	120.3071726	145.975371	11.00436406	59.79866084	17.63392866
naphthacene	119.3466425	142.4162649	10.73293752	58.98543716	17.51660492
benzo[a]pyrene	138.6265448	171.9377027	11.88615146	68.75291488	19.663626
benzo[e]pyrene	138.980392	173.1511395	11.968383	69.0275164	19.70925226
perylene	138.6322575	172.7360981	11.92141296	68.8410981	19.65086524
anthanthrene	157.1999188	199.0184151	12.84595526	77.9230897	21.72263282
benzo[ghi]perylene	157.7417941	200.4576275	12.96364	78.3070707	21.80152768
dibenz[a,h]anthracene	149.3608255	181.8429423	13.19513984	74.00097546	21.59409952
dibenz[a,j]anthracene	149.3550484	181.8379413	13.19465794	73.99885664	21.59297574
picene	149.4560946	182.828113	13.25553356	74.17382468	21.58840548
coronene	176.7264448	228.0341367	13.99040304	87.7029565	23.932869
benzo[c]phenanthrene	120.0446027	144.813816	10.92277414	59.58047692	17.59982112
pyrene	109.3781103	134.1265577	9.57480866	54.24289752	15.70171248
dibenzo[a,c]pyrene	168.2811292	211.0086761	14.2860341	83.5609218	23.68110442
dibenzo[a,h]pyrene	167.8228038	209.6965739	14.19295356	83.2386974	23.61725374
dibenzo[a,i]pyrene	167.9442167	209.812108	14.20516854	83.29423526	23.63823036
dibenzo[a,l]pyrene	168.1274736	210.8264471	14.2681869	83.49379448	23.65114054

(ZE_2), Randić energy (RE), reciprocal Randić energy (RRE), and the atom-bond connectivity energy ($ABCE$) with some thermodynamic properties of polycyclic aromatic compounds namely entropy (S), boiling point (BP), enthalpy of formation (ΔH_f), Kovats retention index (RI), acentric factor (ω), and the octanol-water partition coefficient ($\log P$). The experimental values of benzenoid hydrocarbons (data) are taken from [35, 36]. The molecular graphs of sample compounds are depicted in Figure 1. We computed first Zagreb energy, second Zagreb energy, Randić energy, reciprocal Randić energy, and the atom-bond connectivity energy of benzenoid hydrocarbons by using their definition are shown in Table 1. In this paper, we considered the following linear regression model

$$Y = \theta X + c. \quad (1)$$

Where, Y is dependent variable (property), X is independent variable (topological index), θ is the slope, and c is the intercept respectively. Subsequently, we derived the models in predicting S , BP , (ΔH_f), ω , RI , and $\log P$ of molecules with the help of extended energy of graphs such as the ZE_1 , ZE_2 , RE , RRE , and $ABCE$.

3.2. Models using ZE_1

Using, least square fitting procedure method we found the models of S , ΔH_f , BP , ω , $\log P$, and RI with respect to the first Zagreb energy (ZE_1). Throughout in this paper, the symbols ξ_e , \mathcal{F} , \mathcal{SF} and K are stands for standard error of the

estimate, \mathcal{F} -values, significance \mathcal{F} , and population respectively.

$$BP = 3.2728 \times ZE_1 + 38.605 \quad (2)$$

$$K = 22, \xi_e = 10.60925, \mathcal{F} = 1804.60193, \mathcal{SF} = 4.43396 \times 10^{-21}$$

$$S = 0.3829 \times ZE_1 + 59.027 \quad (3)$$

$$K = 22, \xi_e = 4.51578, \mathcal{F} = 136.36904, \mathcal{SF} = 2.19612 \times 10^{-10}$$

$$\omega = 0.0021 \times ZE_1 + 0.1963 \quad (4)$$

$$K = 11, \xi_e = 0.01879, \mathcal{F} = 124.21539, \mathcal{SF} = 1.44126 \times 10^{-06}$$

$$\log P = 0.0376 \times ZE_1 + 1.077 \quad (5)$$

$$K = 22, \xi_e = 0.19709, \mathcal{F} = 689.67322, \mathcal{SF} = 5.64094 \times 10^{-17}$$

$$\Delta H_f = 1.6383 \times ZE_1 + 66.475 \quad (6)$$

$$K = 22, \xi_e = 16.58967, \mathcal{F} = 184.93809, \mathcal{SF} = 1.4463 \times 10^{-11}$$

$$RI = 3.19 \times ZE_1 + 12.15 \quad (7)$$

$$K = 22, \xi_e = 9.75147, \mathcal{F} = 2029.28791, \mathcal{SF} = 1.38741 \times 10^{-21}$$

3.3. Models corresponding to ZE_2

Corresponding to second Zagreb energy ZE_2 , here we found the models of S , ΔH_f , BP , ω , $\log P$, and RI of polycyclic aromatic compounds.

$$BP = 2.4038 \times ZE_2 + 80.775 \quad (8)$$

$$K = 22, \xi_e = 14.82192, \mathcal{F} = 914.82186, \mathcal{SF} = 3.575 \times 10^{-18}$$

$$S = 0.2772 \times ZE_2 + 64.644 \quad (9)$$

$$K = 22, \xi_e = 5.08249, \mathcal{F} = 103.44187, \mathcal{SF} = 2.37855 \times 10^{-09}$$

$$\omega = 0.0015 \times ZE_2 + 0.2268 \quad (10)$$

$$K = 11, \xi_e = 0.02265, \mathcal{F} = 82.67386, \mathcal{SF} = 7.85218 \times 10^{-06}$$

$$\log P = 0.0276 \times ZE_2 + 1.5664 \quad (11)$$

$$K = 22, \xi_e = 0.23633, \mathcal{F} = 473.57326, \mathcal{SF} = 2.14257 \times 10^{-15}$$

$$\Delta H_f = 1.1852 \times ZE_2 + 90.604 \quad (12)$$

$$K = 22, \xi_e = 19.42251, \mathcal{F} = 129.51593, \mathcal{SF} = 3.4483 \times 10^{-10}$$

$$RI = 2.3398 \times ZE_2 + 53.786 \quad (13)$$

$$K = 22, \xi_e = 14.92859, \mathcal{F} = 854.39091, \mathcal{SF} = 6.9792 \times 10^{-18}$$

3.4. Models using RE

With respect to the Randić energy, here we found the models of S , ΔH_f , BP , ω , $\log P$, and RI of molecules.

$$BP = 45.409 \times RE - 53.855 \quad (14)$$

$$K = 22, \xi_e = 12.75186, \mathcal{F} = 1242.96252, \mathcal{SF} = 1.76012 \times 10^{-19}$$

$$S = 5.5209 \times RE + 45.758 \quad (15)$$

$$K = 22, \xi_e = 3.17043, \mathcal{F} = 297.23313, \mathcal{SF} = 1.80026 \times 10^{-13}$$

$$\omega = 0.0307 \times RE + 0.1239 \quad (16)$$

$$K = 11, \xi_e = 0.01005, \mathcal{F} = 456.52652, \mathcal{SF} = 5.06506 \times 10^{-09}$$

$$\log P = 0.5233 \times RE - 0.0063 \quad (17)$$

$$K = 22, \xi_e = 0.19005, \mathcal{F} = 743.17906, \mathcal{SF} = 2.7244 \times 10^{-17}$$

$$\Delta H_f = 23.476 \times RE + 11.397 \quad (18)$$

$$K = 22, \xi_e = 10.90591, \mathcal{F} = 454.21386, \mathcal{SF} = 3.19925 \times 10^{-15}$$

$$RI = 44.422 \times RE - 79.883 \quad (19)$$

$$K = 22, \xi_e = 8.49367, \mathcal{F} = 2681.17114, \mathcal{SF} = 8.75476 \times 10^{-23}$$

3.5. Models using *RRE*

Here, we found the models of S , ΔH_f , BP , ω , $\log P$, and RI corresponding to the reciprocal Randić energy.

$$BP = 6.5898 \times RRE + 39.145 \quad (20)$$

$$K = 22, \xi_e = 10.76529, \mathcal{F} = 1752.08985, \mathcal{SF} = 5.93856 \times 10^{-21}$$

$$S = 0.7711 \times RRE + 59.089 \quad (21)$$

$$K = 22, \xi_e = 4.52027, \mathcal{F} = 136.0584, \mathcal{SF} = 2.24052 \times 10^{-10}$$

$$\omega = 0.0043 \times RRE + 0.1967 \quad (22)$$

$$K = 11, \xi_e = 0.01888, \mathcal{F} = 122.88936, \mathcal{SF} = 1.50807 \times 10^{-06}$$

$$\log P = 0.0757 \times RRE + 1.0829 \quad (23)$$

$$K = 22, \xi_e = 0.19776, \mathcal{F} = 684.86053, \mathcal{SF} = 6.03869 \times 10^{-17}$$

$$\Delta H_f = 3.2963 \times RRE + 66.908 \quad (24)$$

$$K = 22, \xi_e = 16.72643, \mathcal{F} = 181.60059, \mathcal{SF} = 1.70576 \times 10^{-11}$$

$$RI = 6.4229 \times RRE + 12.682 \quad (25)$$

$$K = 22, \xi_e = 9.92359, \mathcal{F} = 1958.81414, \mathcal{SF} = 1.96903 \times 10^{-21}$$

3.6. Models corresponding to *ABCE*

Here, we found the models of S , ω , $\log P$, BP , ΔH_f , and RI using the atom-bond connectivity energy.

$$BP = 25.59 \times ABCE - 14.028 \quad (26)$$

$$K = 22, \xi_e = 9.04415, \mathcal{F} = 2490.74179, \mathcal{SF} = 1.8191 \times 10^{-22}$$

$$S = 3.0561 \times ABCE + 51.668 \quad (27)$$

$$K = 22, \xi_e = 3.76043, \mathcal{F} = 205.49703, \mathcal{SF} = 5.53548 \times 10^{-12}$$

$$\omega = 0.017 \times ABCE + 0.1559 \quad (28)$$

$$K = 11, \xi_e = 0.01360, \mathcal{F} = 245.31945, \mathcal{SF} = 7.74547 \times 10^{-08}$$

$$\log P = 0.2944 \times ABCE + 0.4628 \quad (29)$$

$$K = 22, \xi_e = 0.17373, \mathcal{F} = 893.35852, \mathcal{SF} = 4.51079 \times 10^{-18}$$

$$\Delta H_f = 13.052 \times ABCE + 35.426 \quad (30)$$

$$K = 22, \xi_e = 13.03449, \mathcal{F} = 311.97855, \mathcal{SF} = 1.14139 \times 10^{-13}$$

$$RI = 24.991 \times ABCE - 40.096 \quad (31)$$

$$K = 22, \xi_e = 5.29089, \mathcal{F} = 6941.21652, \mathcal{SF} = 6.76106 \times 10^{-27}$$

Table 2: Correlation of ZE_1 , ZE_2 , RE , RRE , and $ABCE$ with BP , RI , ω , $\log P$, ΔH_f , and S of benzenoid hydrocarbons

Properties	BP	S	ω	$\log P$	ΔH_f	RI
ZE_1	0.994504251	0.933861578	0.965629453	0.985808305	0.949952396	0.995108292
ZE_2	0.989244939	0.915412709	0.949645137	0.979530075	0.930717461	0.988497312
RE	0.992050511	0.967964298	0.990286348	0.986809926	0.97868531	0.996291024
RRE	0.994340933	0.933725253	0.965277674	0.985710704	0.949101651	0.994933634
$ABCE$	0.99600915	0.954624029	0.982146342	0.988990796	0.969409689	0.998562436

4. DISCUSSIONS

We have seen that, all of these five extended energy of graphs such as ZE_1 , ZE_2 , RE , RRE , and $ABCE$ are well correlated to the Kovats retention index (RI), boiling point (BP), enthalpy of formation (ΔH_f), entropy (S), acentric factor (ω), and octanol-water partition coefficient ($\log P$) of molecules. We have seen that from the above study, the Randić energy is the best descriptor to predict entropy (S), acentric factor (ω), and enthalpy of formation (ΔH_f). Atom-bond connectivity energy is the best for predicting the boiling point (BP), octanol-water partition coefficient ($\log P$), and Kovats retention index (RI). The correlation coefficients of ZE_1 , ZE_2 , RE , RRE , and $ABCE$ with RI , BP , ΔH_f , S , ω , and $\log P$ are already mentioned in Table 2. The scatter diagram of the Kovats retention index (RI), boiling point (BP), enthalpy of formation (ΔH_f), entropy (S), acentric factor (ω), and octanol-water partition coefficient ($\log P$) corresponding to the Randić energy are given in Figure 2. The scatter diagram with respect to ZE_1 , ZE_2 , RRE , and $ABCE$ can be drawn similarly.

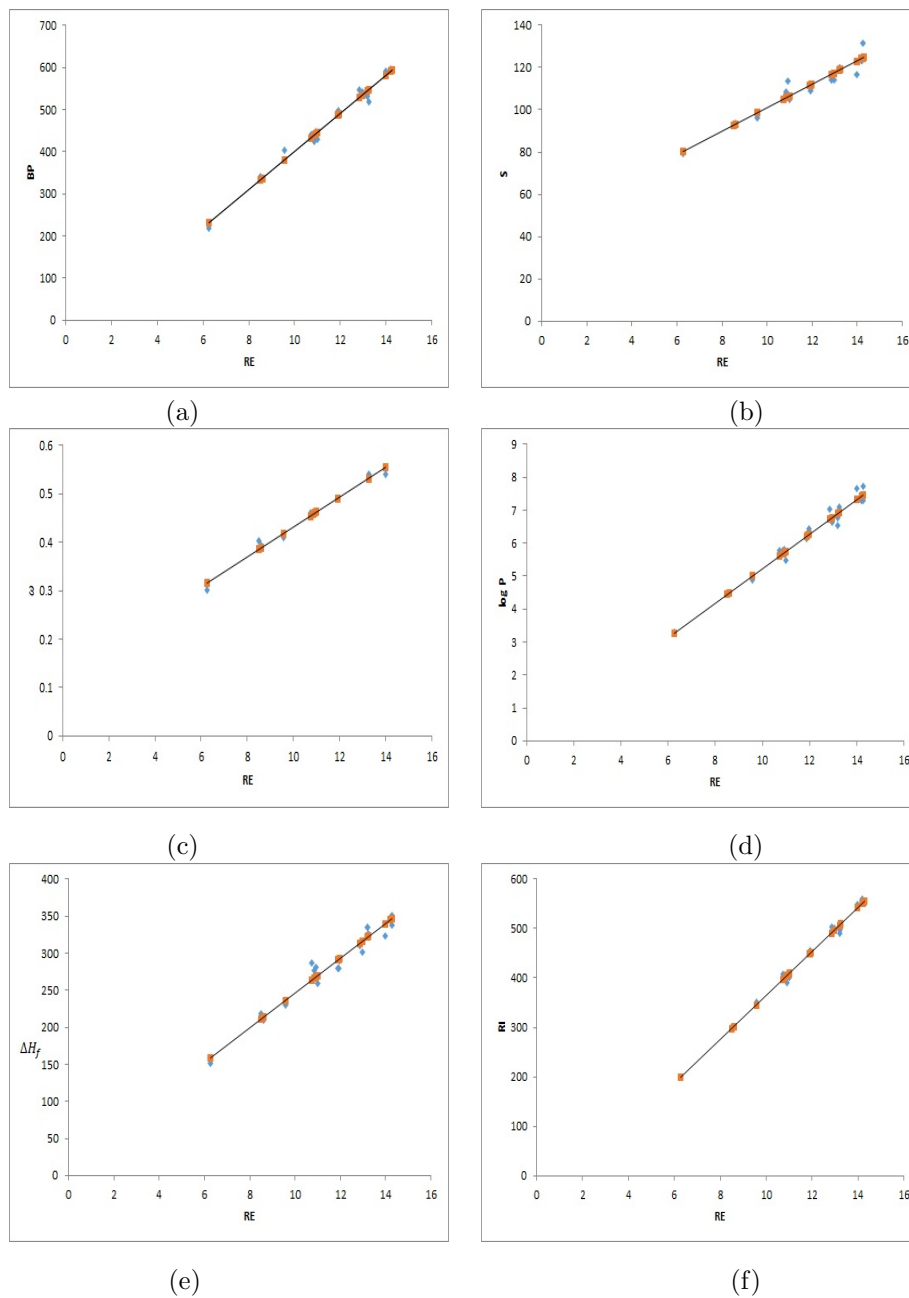


Figure 2: Graphical representation of correlation between RE and BP , RI , $\log P$, ω , ΔH_f , and S . Red dots: predicted y ; blue dots: experimental y .

5. CONCLUSION

In this paper, we dealt with some well-known extended energy of graphs such as ZE_1 , ZE_2 , RE , RRE , and $ABCE$. We mainly, studied their predictive potential of physiochemical properties of polycyclic aromatic compounds with help of a data set of 22-benzenoid hydrocarbons. we established the models of Kovats retention index (RI), boiling point (BP), enthalpy of formation (ΔH_f), entropy (S), acentric factor (ω), and octanol-water partition coefficient ($\log P$) with respect to ZE_1 , ZE_2 , RE , RRE , and $ABCE$. We have seen that these topological indices are well correlated to the properties of RI , BP , ΔH_f , S , ω , and $\log P$ of molecules. Nowadays, a huge number of eigenvalue-based molecular descriptors are available. The significance of some of them is not yet clear. How they can help in chemical sciences or in QSPR or QSAR studies can be discussed comparatively. Also, their mathematical properties such as bounds, minimum, and maximum values, etc. can be discussed. It is also possible to study the topological indices mentioned earlier for different graph operations and other classes of graphs that are not covered in this study.

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Data availability. The data on benzenoid hydrocarbons are taken from [35, 36].

Authors contributions. In this article, all authors have contributed equally.

References

- [1] S. Shanmugam, T. P. Aishwarya, and N. Shreya, "Bridge domination in fuzzy graphs," *Journal of Fuzzy Extension and Applications*, vol. 4, pp. 148–154, 2023.
- [2] R. Jaikumar, R. Sundareswaran, M. Shanmugapriya, S. Broumi, and T. A. Al-Hawary, "Vulnerability parameters in picture fuzzy soft graphs and their applications to locate a diagnosis center in cities," *Journal of Fuzzy Extension and Applications*, vol. 5, no. 1, pp. 86–99, 2024.
- [3] O. Manjusha, "Global domination in fuzzy graphs using strong arcs," *Journal of Fuzzy Extension and Applications*, vol. 4, no. 1, pp. 8–17, 2023.
- [4] R. Kumar, S. Edaltpanah, S. Jha, S. Broumi, and A. Dey, "Neutrosophic shortest path problem," *Neutrosophic Sets and Systems*, vol. 23, pp. 5–15, 2018.
- [5] R. Kumar, S. Edalatpanah, S. Jha, S. Broumi, R. Singh, and A. Dey, "A multi objective programming approach to solve integer valued neutrosophic shortest path problems," *Neutrosophic Sets and Systems*, vol. 24, pp. 134–149, 2019.
- [6] Z. Khodaverdian, H. Sadr, S. A. Edalatpanah, and M. Nazari, "An energy aware resource allocation based on combination of cnn and gru for virtual machine selection," *Multimedia Tools and Applications*, vol. 83, no. 9, pp. 25 769–25 796, 2024.
- [7] H. Wiener, "Structural determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.
- [8] E. Estrada and E. Uriarte, "Recent advances on the role of topological indices in drug discovery research," *Current Medicinal Chemistry*, vol. 8, no. 13, pp. 1573–1588, 2001.
- [9] S. C. Basak, D. Mills, B. D. Gute, G. D. Grunwald, and A. T. Balaban, "Applications of topological indices in the property/bioactivity/toxicity prediction of chemicals," in: *Topology in Chemistry*, Elsevier, pp. 113–184, 2002.

- [10] R. Natarajan, P. Kamalakanan, and I. Nirdosh, "Applications of topological indices to structure-activity relationship modelling and selection of mineral collectors," *Indian Journal of Chemistry. Section A: Inorganic, Physical, Theoretical & Analytical*, vol. 42, no. 6, pp. 1330–1346, 2003.
- [11] H. S. Ramane and A. S. Yalnak, "Status connectivity indices of graphs and its applications to the boiling point of benzenoid hydrocarbons," *Journal of Applied Mathematics and Computing*, vol. 55, no. 1-2, pp. 609–627, 2017.
- [12] I. Gutman and N. Trinajstić, "Graph theory and molecular orbitals. total φ -electron energy of alternant hydrocarbons," *Chemical Physics Letters*, vol. 17, no. 4, pp. 535–538, 1972.
- [13] M. Randić, "Characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, no. 23, pp. 6609–6615, 1975.
- [14] O. Favaron, M. Mahéo, and J.-F. Saclé, "Some eigenvalue properties in graphs (conjectures of graffiti—ii)," *Discrete Mathematics*, vol. 111, no. 1-3, pp. 197–220, 1993.
- [15] E. Estrada, L. Torres, L. Rodriguez, and I. Gutman, "An atom-bond connectivity index: modelling the enthalpy of formation of alkanes," *Indian Journal of Chemistry. Section A: Inorganic, Physical, Theoretical & Analytical*, vol. 37A, pp. 849–855, 1998.
- [16] I. Gutman and J. Tošović, "Testing the quality of molecular structure descriptors. vertex-degree-based topological indices," *Journal of the Serbian Chemical Society*, vol. 78, no. 6, pp. 805–810, 2013.
- [17] M. Randić, "On history of the randić index and emerging hostility toward chemical graph theory," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 59, pp. 5–124, 2008.
- [18] K. C. Das, "Atom-bond connectivity index of graphs," *Discrete Applied Mathematics*, vol. 158, no. 11, pp. 1181–1188, 2010.
- [19] I. Gutman, J. Tošović, S. Radenković, and S. Marković, "On atom-bond connectivity index and its chemical applicability," *Indian Journal of Chemistry*, vol. 51, no. 5, pp. 690–694, 2012.
- [20] I. Gutman, "Degree-based topological indices," *Croatica Chemica Acta*, vol. 86, no. 4, pp. 351–361, 2013.
- [21] M. Imran, S. Hayat, and M. Y. H. Mailk, "On topological indices of certain interconnection networks," *Applied Mathematics and Computation*, vol. 244, pp. 936–951, 2014.
- [22] F. Chaudhry, M. N. Husin, F. Afzal, D. Afzal, M. Ehsan, M. Cancan, and M. R. Farahani, "M-polynomials and degree-based topological indices of tadpole graph," *Journal of Discrete Mathematical Sciences and Cryptography*, vol. 24, no. 7, pp. 2059–2072, 2021.
- [23] M. N. Husin, S. Zafar, and R. Gobithaasan, "Investigation of atom-bond connectivity indices of line graphs using subdivision approach," *Mathematical Problems in Engineering*, vol. 2022, pp. 1–9, 2022.
- [24] B. Zhou and N. Trinajstić, "Mathematical properties of molecular descriptors based on distances," *Croatica Chemica Acta*, vol. 83, no. 2, pp. 227–242, 2010.
- [25] K. C. Das, I. Gutman, I. Milovanović, E. Milovanović, and B. Furtula, "Degree-based energies of graphs," *Linear Algebra and its Applications*, vol. 554, pp. 185–204, 2018.
- [26] I. Gutman, B. Furtula, and K. C. Das, "Extended energy and its dependence on molecular structure," *Canadian Journal of Chemistry*, vol. 95, no. 5, pp. 526–529, 2017.
- [27] M. Akram, S. Naz, S. Shahzadi, and F. Ziaa, "Geometric-arithmetic energy and atom bond connectivity energy of dual hesitant q-rung orthopair fuzzy graphs," *Journal of Intelligent & Fuzzy Systems*, vol. 40, no. 1, pp. 1287–1307, 2021.
- [28] S. Hayat, S. Khan, and M. Imran, "Quality testing of spectrum-based distance descriptors for polycyclic aromatic hydrocarbons with applications to carbon nanotubes and nanocones," *Arabian Journal of Chemistry*, vol. 14, no. 3, p. 102994, 2021.
- [29] M. Akram, D. Saleem, and B. Davvaz, "Energy of double dominating bipolar fuzzy graphs," *Journal of Applied Mathematics and Computing*, vol. 61, pp. 219–234, 2019.
- [30] M. Akram and S. Naz, "Energy of pythagorean fuzzy graphs with applications," *Mathematics*, vol. 6, no. 8, p. 136, 2018.
- [31] S. Hayat and S. Khan, "Quality testing of spectrum-based valency descriptors for polycyclic aromatic hydrocarbons with applications," *Journal of Molecular Structure*, vol. 1228, no. 129789, pp. 1–15, 2021.

- [32] N. J. Rad, A. Jahanbani, and I. Gutman, "Zagreb energy and zagreb estrada index of graphs," *MATCH-Communications in Mathematical and in Computer Chemistry*, vol. 79, no. 2018, 2018.
- [33] S. B. Bozkurt, A. D. Güngör, I. Gutman, and A. S. Cevik, "Randic matrix and randic energy," *MATCH-Communications in Mathematical and in Computer Chemistry*, vol. 64, no. 1, pp. 239–250, 2010.
- [34] E. Estrada, "The abc matrix," *Journal of Mathematical Chemistry*, vol. 55, pp. 1021–1033, 2017.
- [35] P. Sarkar, N. De, and A. Pal, "On some topological indices and their importance in chemical sciences: a comparative study," *The European Physical Journal Plus*, vol. 137, no. 195, pp. 1–12, 2022.
- [36] S. Kumar, P. Sarkar, and A. Pal, "A study on the energy of graphs and its applications," *Polycyclic Aromatic Compounds*, pp. 1–10, 2023.