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# ON SOME EXTENDED ENERGY OF GRAPHS AND THEIR APPLICATIONS

Prosanta SARKAR
*Department of Basic Science & Humanities (Mathematics), Ramgarh Engineering College, Ramgarh, Jharkhand, India*
*prosantasarkar87@gmail.com*

Arindam DEY*
*School of Computer Science & Engineering,VIT-AP University, Amaravati, Andhra Pradesh, India, arindam84nit@gmail.co*

Shiv KUMAR
*Department of Basic Science & Humanities (Mathematics), Ramgarh Engineering College, Ramgarh, Jharkhand, India*
*dr.shivkumar276403@gmail.com*

Anita PAL
*Department of Mathematics, National Institute of Technology Durgapur, Durgapur, West Bengal, India, anita.pal@maths.nitdgp.ac.in*

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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 ($\Delta H_f$), octanol-water partition coefficient ($logP$), and acentric factor ($\omega$) of benzenoid hydrocarbons.

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

**MSC:** 05C35, 05C07, 05C40.

*Corresponding author

## 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 $V(G) = \{v_1, v_2, v_3, \cdots, v_n\}$. If the two vertices $v_i$ and $v_j$ are connected by a line (adjacent), we denote it as $v_iv_j \in E(G)$. 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 topological indices are defined as

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

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

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

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

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

The extended energy of $G$ is defined as

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

where, $\eta_1, \eta_2, \cdots, \eta_n$ 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

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

and

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

Suppose $\eta_1^{(1)}, \eta_2^{(1)}, \cdots, \eta_n^{(1)}$ and $\eta_1^{(2)}, \eta_2^{(2)}, \cdots, \eta_n^{(2)}$ 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, $i = 1, 2, \cdots, n$. The Randić matrix and reciprocal Randić matrix are defined as

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

and

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

If the $\zeta_i^{'}$ and $\zeta_i^{''}$, $i = 1, 2, \cdots, n$ 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

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

If $\xi_i$, $i = 1, 2, \cdots, n$ 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.

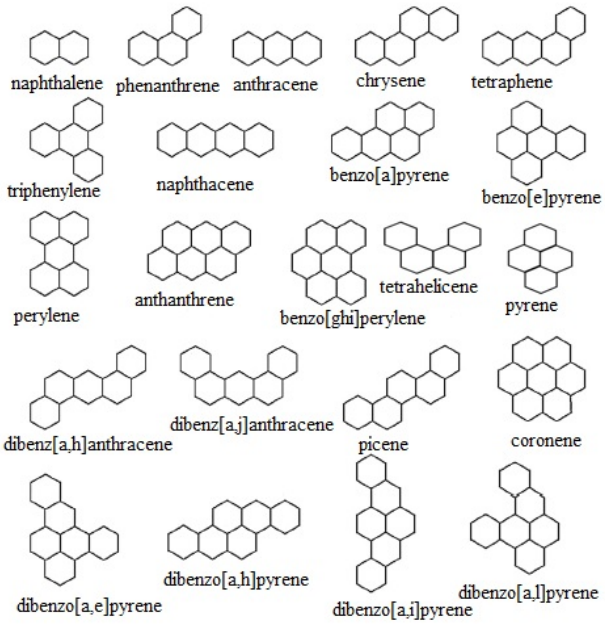



Figure 1: Molecular graphs of benzenoid hydrocarbons

## 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 ($ZE_2$), 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 ($\Delta H_f$), Kovats retention index ($RI$), acentric factor ($\omega$), and the octanol-water partition coefficient ($logP$). 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

Table 1: Energies of benzenoid hydrocarbons

| MoleculesEnergies | $ZE_1$ | $ZE_2$ | $RE$ | $RRE$ | $ABCE$ |
|---|---|---|---|---|---|
| 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,e]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 |

of benzenoid hydrocarbons by using their definition are shown in Table 1. In this paper, we considered the following linear regression model

$$Y = \theta X + c. \tag{1}$$

Where, $Y$ is dependent variable (property), X is independent variable (topological index), $\theta$ is the slope, and $c$ is the intercept respectively. Subsequently, we derived the models in predicting $S$, $BP$, $(\Delta H_f)$, $\omega$, $RI$, and $logP$ 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 $S$, $\Delta H_f$, $BP$, $\omega$, $\log P$, and $RI$ with respect to the first Zagreb energy ($ZE_1$). Throughout in this paper, the symbols $\xi_e$, $\mathcal{F}$, $\mathcal{SF}$ and $K$ are stands for standard error of the estimate, $\mathcal{F}$-values, significance $\mathcal{F}$, and population respectively.

$$\begin{aligned} BP &= 3.2728 \times ZE_1 + 38.605 \qquad (2)\\ &\quad K = 22, \xi_e = 10.60925, \mathcal{F} = 1804.60193, \mathcal{SF} = 4.43396 \times 10^{-21} \\ S &= 0.3829 \times ZE_1 + 59.027 \qquad (3)\\ &\quad K = 22, \xi_e = 4.51578, \mathcal{F} = 136.36904, \mathcal{SF} = 2.19612 \times 10^{-10} \\ \omega &= 0.0021 \times ZE_1 + 0.1963 \qquad (4)\\ &\quad K = 11, \xi_e = 0.01879, \mathcal{F} = 124.21539, \mathcal{SF} = 1.44126 \times 10^{-06} \end{aligned}$$

$$\begin{aligned} logP &= 0.0376 \times ZE_1 + 1.077 \quad (5)\\ &\quad K = 22, \xi_e = 0.19709, \mathcal{F} = 689.67322, \mathcal{SF} = 5.64094 \times 10^{-17}\\ \Delta H_f &= 1.6383 \times ZE_1 + 66.475 \quad (6)\\ &\quad K = 22, \xi_e = 16.58967, \mathcal{F} = 184.93809, \mathcal{SF} = 1.4463 \times 10^{-11}\\ RI &= 3.19 \times ZE_1 + 12.15 \quad (7)\\ &\quad K = 22, \xi_e = 9.75147, \mathcal{F} = 2029.28791, \mathcal{SF} = 1.38741 \times 10^{-21} \end{aligned}$$

### 3.3. Models corresponding to $ZE_2$

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

$$\begin{aligned} BP &= 2.4038 \times ZE_2 + 80.775 \quad (8)\\ &\quad K = 22, \xi_e = 14.82192, \mathcal{F} = 914.82186, \mathcal{SF} = 3.575 \times 10^{-18}\\ S &= 0.2772 \times ZE_2 + 64.644 \quad (9)\\ &\quad K = 22, \xi_e = 5.08249, \mathcal{F} = 103.44187, \mathcal{SF} = 2.37855 \times 10^{-09}\\ \omega &= 0.0015 \times ZE_2 + 0.2268 \quad (10)\\ &\quad K = 11, \xi_e = 0.02265, \mathcal{F} = 82.67386, \mathcal{SF} = 7.85218 \times 10^{-06}\\ logP &= 0.0276 \times ZE_2 + 1.5664 \quad (11)\\ &\quad K = 22, \xi_e = 0.23633, \mathcal{F} = 473.57326, \mathcal{SF} = 2.14257 \times 10^{-15}\\ \Delta H_f &= 1.1852 \times ZE_2 + 90.604 \quad (12)\\ &\quad K = 22, \xi_e = 19.42251, \mathcal{F} = 129.51593, \mathcal{SF} = 3.4483 \times 10^{-10}\\ RI &= 2.3398 \times ZE_2 + 53.786 \quad (13)\\ &\quad K = 22, \xi_e = 14.92859, \mathcal{F} = 854.39091, \mathcal{SF} = 6.9792 \times 10^{-18} \end{aligned}$$

### 3.4. Models using $RE$

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

$$\begin{aligned} BP &= 45.409 \times RE - 53.855 \quad (14)\\ &\quad K = 22, \xi_e = 12.75186, \mathcal{F} = 1242.96252, \mathcal{SF} = 1.76012 \times 10^{-19}\\ S &= 5.5209 \times RE + 45.758 \quad (15)\\ &\quad K = 22, \xi_e = 3.17043, \mathcal{F} = 297.23313, \mathcal{SF} = 1.80026 \times 10^{-13}\\ \omega &= 0.0307 \times RE + 0.1239 \quad (16)\\ &\quad K = 11, \xi_e = 0.01005, \mathcal{F} = 456.52652, \mathcal{SF} = 5.06506 \times 10^{-09}\\ logP &= 0.5233 \times RE - 0.0063 \quad (17)\\ &\quad K = 22, \xi_e = 0.19005, \mathcal{F} = 743.17906, \mathcal{SF} = 2.7244 \times 10^{-17} \end{aligned}$$

$$\Delta H_f = 23.476 \times RE + 11.397 \quad (18)$$
$$K = 22, \xi_e = 10.90591, \mathcal{F} = 454.21386, \mathcal{SF} = 3.19925 \times 10^{-15}$$
$$RI = 44.422 \times RE - 79.883 \quad (19)$$
$$K = 22, \xi_e = 8.49367, \mathcal{F} = 2681.17114, \mathcal{SF} = 8.75476 \times 10^{-23}$$

### 3.5. Models using *RRE*

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

$$BP = 6.5898 \times RRE + 39.145 \quad (20)$$
$$K = 22, \xi_e = 10.76529, \mathcal{F} = 1752.08985, \mathcal{SF} = 5.93856 \times 10^{-21}$$
$$S = 0.7711 \times RRE + 59.089 \quad (21)$$
$$K = 22, \xi_e = 4.52027, \mathcal{F} = 136.0584, \mathcal{SF} = 2.24052 \times 10^{-10}$$
$$\omega = 0.0043 \times RRE + 0.1967 \quad (22)$$
$$K = 11, \xi_e = 0.01888, \mathcal{F} = 122.88936, \mathcal{SF} = 1.50807 \times 10^{-06}$$
$$logP = 0.0757 \times RRE + 1.0829 \quad (23)$$
$$K = 22, \xi_e = 0.19776, \mathcal{F} = 684.86053, \mathcal{SF} = 6.03869 \times 10^{-17}$$
$$\Delta H_f = 3.2963 \times RRE + 66.908 \quad (24)$$
$$K = 22, \xi_e = 16.72643, \mathcal{F} = 181.60059, \mathcal{SF} = 1.70576 \times 10^{-11}$$
$$RI = 6.4229 \times RRE + 12.682 \quad (25)$$
$$K = 22, \xi_e = 9.92359, \mathcal{F} = 1958.81414, \mathcal{SF} = 1.96903 \times 10^{-21}$$

### 3.6. Models corresponding to *ABCE*

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

$$BP = 25.59 \times ABCE - 14.028 \quad (26)$$
$$K = 22, \xi_e = 9.04415, \mathcal{F} = 2490.74179, \mathcal{SF} = 1.8191 \times 10^{-22}$$
$$S = 3.0561 \times ABCE + 51.668 \quad (27)$$
$$K = 22, \xi_e = 3.76043, \mathcal{F} = 205.49703, \mathcal{SF} = 5.53548 \times 10^{-12}$$
$$\omega = 0.017 \times ABCE + 0.1559 \quad (28)$$
$$K = 11, \xi_e = 0.01360, \mathcal{F} = 245.31945, \mathcal{SF} = 7.74547 \times 10^{-08}$$
$$logP = 0.2944 \times ABCE + 0.4628 \quad (29)$$
$$K = 22, \xi_e = 0.17373, \mathcal{F} = 893.35852, \mathcal{SF} = 4.51079 \times 10^{-18}$$
$$\Delta H_f = 13.052 \times ABCE + 35.426 \quad (30)$$
$$K = 22, \xi_e = 13.03449, \mathcal{F} = 311.97855, \mathcal{SF} = 1.14139 \times 10^{-13}$$
$$RI = 24.991 \times ABCE - 40.096 \quad (31)$$
$$K = 22, \xi_e = 5.29089, \mathcal{F} = 6941.21652, \mathcal{SF} = 6.76106 \times 10^{-27}$$

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

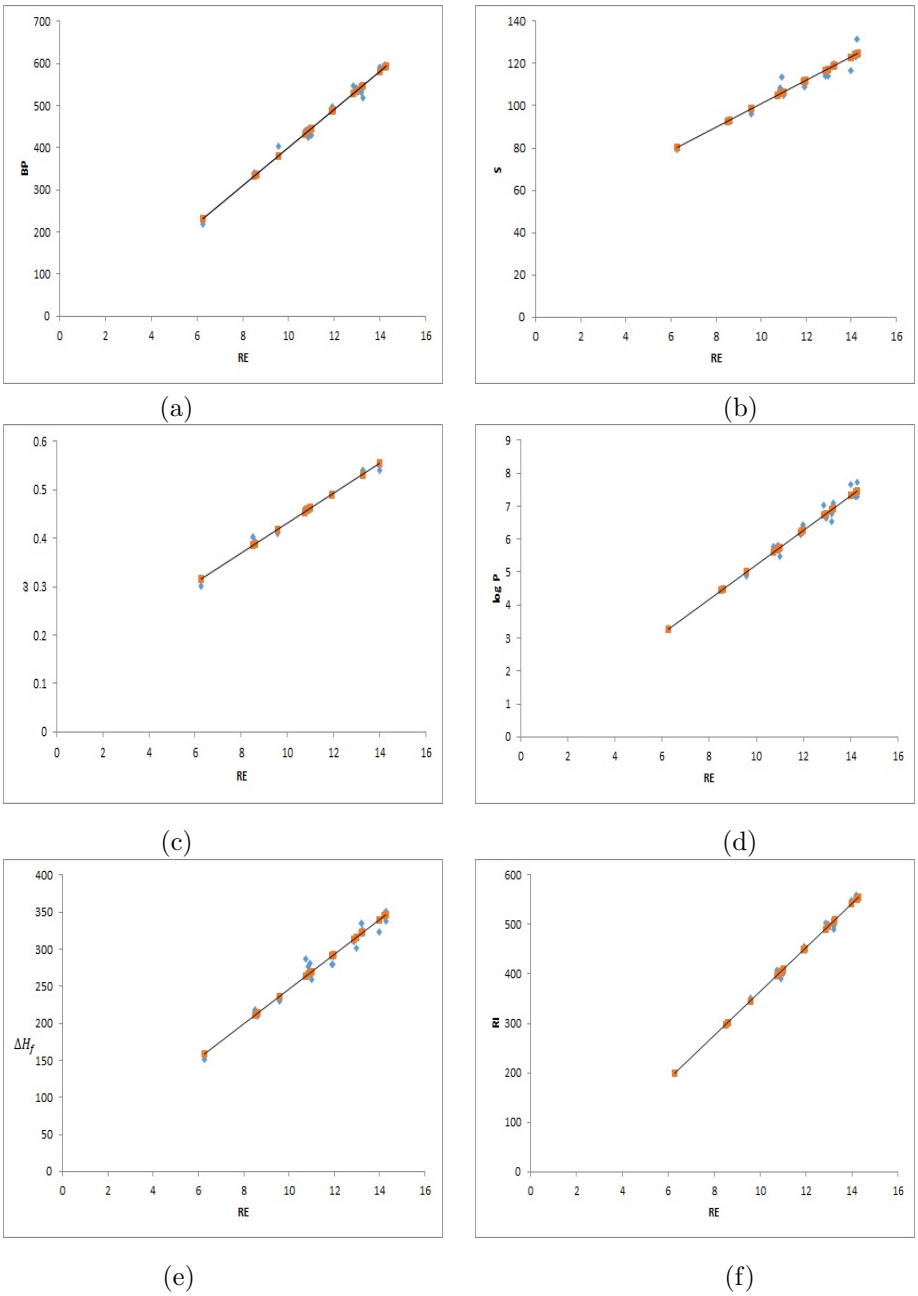
| EnergiesProperties | $BP$ | $S$ | $\omega$ | $\log P$ | $\Delta H_f$ | $RI$ |
|---|---|---|---|---|---|---|
| $ZE_1$ | 0.994504251 | 0.933861578 | 0.965629453 | 0.985808305 | 0.949952396 | 0.995108292 |
| $ZE_2$ | 0.989244939 | 0.915412709 | 0.949645137 | 0.979530075 | 0.930717461 | 0.988497312 |
| $RE$ | 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 ($\Delta H_f$), entropy ($S$), acentric factor ($\omega$), and octanol-water partition coefficient ($logP$) of molecules. We have seen that from the above study, the Randić energy is the best descriptor to predict entropy ($S$), acentric factor ($\omega$), and enthalpy of formation ($\Delta H_f$). Atom-bond connectivity energy is the best for predicting the boiling point ($BP$), octanol-water partition coefficient ($logP$), and Kovats retention index ($RI$). The correlation coefficients of $ZE_1$, $ZE_2$, $RE$, $RRE$, and $ABCE$ with $RI$, $BP$, $\Delta H_f$, $S$, $\omega$, and $\log P$ are already mentioned in Table 2. The scatter diagram of the Kovats retention index ($RI$), boiling point ($BP$), enthalpy of formation ($\Delta H_f$), entropy ($S$), acentric factor ($\omega$), and octanol-water partition coefficient ($logP$) 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.

## 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 ($\Delta H_f$), entropy ($S$), acentric factor ($\omega$), and octanol-water partition coefficient ($logP$) 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 $RI$, $BP$, $\Delta H_f$, $S$, $\omega$, and $logP$ 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.




(a) (b) (c) (d) (e) (f)

Figure 2: Graphical representation of correlation between $RE$ and $BP$, $RI$, $logP$, $\omega$, $\Delta H_f$, and $S$. Red dots: predicted y; blue dots: experimental y.

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

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