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Sarojini Naik¹, Meenal M. Kaliwal²,
Vidya S. Umadi³

¹Research Scholar, Department of Mathematics,
KLS Vishwanathrao Deshpande Institute of
Technology, Haliyal-581329, INDIA.

²Department of Mathematics, KLS Vishwanathrao
Deshpande Institute of Technology, Haliyal
581329, Karnataka State, India.

³Department of Mathematics, East Point College
of Engineering and Technology, Bengaluru
581329, Karnataka State, India.

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Sarojini Naik^{1*}, Meenal M. Kaliwal², Vidya S. Umadi³

¹Research Scholar, Department of Mathematics, KLS Vishwanathrao Deshpande Institute of Technology, Haliyal-581329, INDIA.

²Department of Mathematics, KLS Vishwanathrao Deshpande Institute of Technology, Haliyal 581329, Karnataka State, India.

³Department of Mathematics, East Point College of Engineering and Technology, Bengaluru 581329, Karnataka State, India.

Contributing authors: sarojini.naik22@gmail.com; mmk@klsvidit.edu.in

Abstract

Let G be a simple graph of order n and size m , the vertex weight and edge weight is defined as $w(v_i) = d_G(v_i)$ and $w(e_i) = d_G(v_i) + d_G(v_j) - 2$ for $e = v_i v_j$. The edge mass adjacency matrix $A_w(G)$ of a graph G is defined in such a way that, for any v_i that is adjacent to v_j , its (i, j) -entry equals $d_G(v_i) + d_G(v_j) - 2$; otherwise, it equals 0. We look at the $A_w(G)$'s spectral radius λ_1^w and energy $E_w(G)$. Lower and upper bounds are obtained for λ_1^w and $E_w(G)$ and the respective extremal graphs are characterised. Further we consider a set of 22 benzenoid hydrocarbons and calculate their graph energy and edge mass energy by drawing its molecular graphs. The correlation between physiochemical properties of benzenoid hydrocarbons, molecular descriptors and graph energies are obtained and regression models are studied to check the predictability of physiochemical properties of benzenoid hydrocarbons with $E(G)$ and $E_w(G)$.

Keywords: Edge weight energy, spectral radius, benzenoid hydrocarbons, molecular descriptors.

1 Introduction

Every graph taken into consideration here is a simple graph $G = (V, E)$, where $|V| = n$ and $|E| = m$. The count of edges connected to a vertex $v \in V$, denoted by $d_G(v)$ is the degree of that vertex. The degree of an edge $e = uv$ is defined by $d_G(e) = d_G(u) + d_G(v) - 2$. $\Delta(\delta)$ and $\Delta'(\delta')$ represents the maximum (minimum) vertex and edge degree of a graph respectively. If $\Delta_G = \delta_G = n - 1$ then the graph G is said to be complete denoted by K_n . In G if $V(G)$ is partitioned into two sets say M and N (partite sets) such that every edge meet both M and N then the graph is bipartite graph. If every vertex of M is adjacent to every vertex of N then the graph is complete bipartite graph denoted as $K_{m,n}$. The graph $K_{1,n-1}$ denoted by S_n is a star graph and the graph $K_{n,n}$ is called equi-bipartite graph. \bar{G} represents the complement of a graph G , which is defined on same vertex set as of G such that if two vertices are adjacent in \bar{G} , then they are not adjacent in G . The positive integer less than or equal to x is $\lfloor x \rfloor$, for any integer x .

The first degree-based molecular descriptor, the Zagreb index, was developed by Gutman and Trinajstić[8]. It firstly emerged in the topological formula for conjugated molecules total π -electron energy, the first Zagreb index is defined as:

$$M_1(G) = \sum_{u \in V} d_G(v)^2 = \sum_{uv \in E(G)} (d_G(u) + d_G(v)) \quad (1)$$

The Zagreb indices were reformulated in 2004 by Milićević et al.[1] in terms of edge degree, where the edge degree is given by $d_G(e) = d_G(u) + d_G(v) - 2$ for $e = uv \in E(G)$. Thus the first reformulated Zagreb index is given by

$$EM_1(G) = \sum_{e \in E(G)} d_G(e)^2 \quad (2)$$

For more terminologies refer the following [1,3,8]. The sum of the absolute values of eigenvalues of the adjacency matrix of G gives us the energy $E(G)$ of a graph G . This quantity is introduced in [9]. Suppose $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ are the eigenvalues of the adjacency matrix $A(G)$ then the energy of the graph G is given by

$$E(G) = \sum_{i=1}^n |\lambda_i| \quad (3)$$

The extended adjacency matrix of graph G was proposed by Yang et al.[19] in 1994, denoted by $A_{ex}(G)$, it was defined as its (i, j) -entry is equal to $\frac{1}{2} \left(\frac{d_j}{d_i} + \frac{d_i}{d_j} \right)$ if $v_i \sim v_j$ and 0 otherwise. Since A_{ex} is a real symmetric matrix of order n , all its eigenvalues are real, which are denoted as $\eta_1 \geq \eta_2 \geq \dots \geq \eta_n$. Yang et al.[19] also investigated the extended graph energy by summing the absolute values of the eigenvalues of the A_{ex} -matrix, defined as

$$E_{ex}(G) = \sum_{i=1}^n |\eta_i| \quad (4)$$

For recent studies on graph energy refer [2,6,11,12,18].

1.1 Edge mass graph energy

For a given graph G , we define the following terminologies:

Definition 1. Let $V = \{v_1, v_2, \dots, v_n\}$ be the vertex set and $\{w_1, w_2, \dots, w_n\}$ be the weights, then the vertex weight for $v_i \in V$ is defined as $w(v_i) = d_G(v_i)$.

Definition 2. Let $E = \{e_1, e_2, \dots, e_m\}$ be the edge set, then the edge weight $e_i = v_i v_j$ is defined by $w(e_i) = d_G(v_i) + d_G(v_j) - 2$.

Definition 3. The mass degree of a vertex $v_i \in V(G)$ is defined as

$$d_G^w(v_i) = \sum_{e_i = v_i v_j} w(e_i)$$

Observe that

$$\sum_{i=1}^n d_G^w(v_i) = 2 \sum_{i=1}^n w(e_i) = 2 \sum_{uv \in E} [d_G(v_i) + d_G(v_j) - 2] = 2[M_1 - 2m]$$

Motivated by the extended adjacency matrix of graph G , we introduce a new edge mass adjacency matrix of graph G denoted by $A_w(G)$. It is defined in such a way that, for any v_i that is adjacent to v_j , its (i, j) -entry equals $d_G(v_i) + d_G(v_j) - 2$; otherwise, it equals 0. In fact, $A_w(G)$ is a real symmetric matrix of order n . Hence all its eigenvalues are real and can be arranged as $\lambda_1^w \geq \lambda_2^w \geq \dots \geq \lambda_n^w$, where the largest eigenvalue λ_1^w is called as the spectral radius of $A_w(G)$. The edge mass graph energy of G is given by

$$E_w = E_w(G) = \sum_{i=1}^n |\lambda_i^w| \tag{5}$$

1.2 Identities

1. $\sum_{i=1}^n \lambda_i^w = 0$
2. $\sum_{i=1}^n (\lambda_i^w)^2 = 2\sum_{i=1}^n [w(e_i)]^2 = 2\sum_{i=1}^n d_G(e_i)^2 = 2EM_1(G)$
3. $\sum_{0 \leq i \leq j} \lambda_i^w \lambda_j^w = -\sum_{i=1}^n [w(e_i)]^2 = -\sum_{i=1}^n d_G(e_i)^2 = -EM_1(G)$

Observe that,

1. $\sum_{i=1}^n (\lambda_i^w)^2 = 2EM_1(G)$
2. $\sum_{0 \leq i \leq j} \lambda_i^w \lambda_j^w = -EM_1(G)$

Examples:

1. The edge mass graph energy of K_n is $4(n - 1)(n - 2)$.
2. The edge mass graph energy of $K_{m,n}$ is $2(m + n - 2)\sqrt{mn}$.
3. The edge mass graph energy of S_n is $2(n - 2)\sqrt{(n - 1)}$.
4. The edge mass graph energy of $K_{n,n}$ is $4n(n - 1)$.

2 Auxiliary Results

In this section, we need the following already established results.

Lemma 2.1 [2]. If C is a real symmetric $n \times n$ matrix with eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$, then for $x \in \mathbb{R}^n$, such that $x \neq 0$,

$$x^T C x \leq \lambda_1 x^T x \tag{6}$$

Lemma 2.2 [2]. Let $C = (c_{ij})$ and $D = (d_{ij})$ be real symmetric non-negative matrices of order n . If $C \geq D$, i.e., $c_{ij} \geq d_{ij}$ for all i, j , then $\lambda_1(C) \geq \lambda_1(D)$, λ_1 is the largest eigenvalue.

Lemma 2.3 [2]. Let G be a connected graph of order n with m edges. Then

$$\lambda_1(G) \leq \sqrt{2m - n + 1} \tag{7}$$

with equality if and only if $G \cong K_{1,n-1}$ or $G \cong K_n$.

Lemma 2.4 [2]. Let G be a connected graph of order $n \geq 2$. Then $\lambda_1 > \lambda_2$

Lemma 2.5 [2]. Let G be a graph of order n . Then $|\lambda_1| = |\lambda_2| = \dots = |\lambda_n|$ if and only if $G \cong \overline{K_n}$ or $G \cong \frac{n}{2}K_2$

Lemma 2.6 [18]. (CauchySchwartz inequality:) Let r_i and $s_i, 1 \leq i \leq n$ be any real numbers, then

$$\left(\sum_{i=1}^n r_i s_i\right)^2 \leq \left(\sum_{i=1}^n r_i^2\right)\left(\sum_{i=1}^n s_i^2\right) \quad (8)$$

Lemma 2.7 [20]. (Chebyshev's inequality:) For real numbers $r_1 \leq r_2 \leq \dots \leq r_n$ and $s_1 \leq s_2 \leq \dots \leq s_n$, then

$$\left(\sum_{i=1}^n r_i\right)\left(\sum_{i=1}^n s_i\right) \leq n \sum_{i=1}^n r_i s_i \quad (9)$$

Lemma 2.8 [16]. (Ozeki inequality:) If r_i and $s_i (1 \leq i \leq n)$ are non-negative real numbers then

$$\sum_{i=1}^n r_i^2 \sum_{i=1}^n s_i^2 - \left[\sum_{i=1}^n r_i s_i\right]^2 \leq \frac{n^2}{4} (P_1 P_2 - p_1 p_2)^2 \quad (10)$$

where $P_1 = \max_{1 \leq i \leq n} \{r_i\}, P_2 = \max_{1 \leq i \leq n} \{s_i\}, p_1 = \min_{1 \leq i \leq n} \{r_i\}, p_2 = \min_{1 \leq i \leq n} \{s_i\}$

Lemma 2.9 [6]. Let p_i, q_i, r_i and s_i are sequences of real numbers and m_i, n_i are non-negative for $i = 1, 2, \dots, n$. Then the following inequality is valid

$$\sum_{i=1}^n m_i p_i^2 \sum_{i=1}^n n_i q_i^2 + \sum_{i=1}^n m_i r_i^2 \sum_{i=1}^n m_i s_i^2 \geq 2 \sum_{i=1}^n m_i p_i r_i \sum_{i=1}^n n_i q_i s_i \quad (11)$$

Lemma 2.10 [6]. Let p_i, q_i are sequences of real numbers and r_i, s_i are non-negative for $i = 1, 2, \dots, n$. Then the following inequality is valid

$$\sum_{i=1}^n s_i \sum_{i=1}^n r_i p_i^2 + \sum_{i=1}^n r_i \sum_{i=1}^n s_i q_i^2 \geq 2 \sum_{i=1}^n r_i s_i \sum_{i=1}^n s_i q_i \quad (12)$$

Lemma 2.11 [18]. Let $r_i, 1 \leq i \leq n$ be any real numbers, then

$$\left(\sum_{i=1}^n |r_i|\right)^2 \geq \left(\sum_{i=1}^n |r_i|^2\right) \quad (13)$$

Lemma 2.12 [5]. Suppose r_i and $s_i, 1 \leq i \leq n$ are positive real numbers, then

$$\sum_{i=1}^n r_i^2 \sum_{i=1}^n s_i^2 \leq \frac{1}{4} \left(\sqrt{\frac{P_1 P_2}{p_1 p_2}} + \sqrt{\frac{p_1 p_2}{P_1 P_2}} \right)^2 \left(\sum_{i=1}^n r_i s_i\right)^2 \quad (14)$$

where $P_1 = \max_{1 \leq i \leq n} \{r_i\}, P_2 = \max_{1 \leq i \leq n} \{s_i\}, p_1 = \min_{1 \leq i \leq n} \{r_i\}, p_2 = \min_{1 \leq i \leq n} \{s_i\}$.

Lemma 2.13 [15]. Suppose r_i and $s_i, 1 \leq i \leq n$ are positive real numbers, then

$$\left| n \sum_{i=1}^n r_i s_i - \sum_{i=1}^n r_i \sum_{i=1}^n s_i \right| \leq \alpha(n)(R-r)(S-s) \quad (15)$$

where r, s, R and S are real constants, that for each $i, 1 \leq i \leq n, r \leq r_i \leq R$ and $s \leq s_i \leq S$.

Further, $\alpha(n) = n \binom{n}{2} \left(1 - \frac{1}{n} \binom{n}{2}\right)$

Lemma 2.14 [10]. Let r_i and $s_i, 1 \leq i \leq n$ are nonnegative real numbers, then

$$\sum_{i=1}^n s_i^2 + pP \sum_{i=1}^n r_i^2 \leq (p+P) \left(\sum_{i=1}^n r_i s_i \right) \quad (16)$$

where p and P are real constants, so that for each $i, 1 \leq i \leq n$, holds, $pr_i \leq s_i \leq Pr_i$.

Lemma 2.15. Let G be a connected graph of order $n \geq 2$, then $\lambda_1^w > \lambda_2^w$

Proof: Let us assume that $\lambda_1^w = \lambda_2^w$. Since G is connected, $A^w(G)$ is an irreducible non-negative $n \times n$ matrix then by Perron-Frobenius theorem, the eigen vector x corresponding to λ_1^w has all components positive. Let y be an eigenvector corresponding to λ_2^w . Since $\lambda_1^w = \lambda_2^w$, any linear combination of x and y would be an eigenvector corresponding to λ_1^w . Then it would be easily adjust that the component of this factor be equal to zero a contradiction.

Lemma 2.16. Let G be a graph of order n then $|\lambda_1^w| = |\lambda_2^w| = \dots = |\lambda_n^w|$ if and only if $G \cong \overline{K_n}$ or $G \cong \frac{n}{2}K_2$.

Proof: First we assume that $|\lambda_1^w| = |\lambda_2^w| = \dots = |\lambda_n^w|$. Let S be the number of isolated vertices in G . If $S \geq 1$ then $\lambda_1^w = \lambda_2^w = \dots = \lambda_n^w = 0$, hence $G \cong \overline{K_n}$ or $G \cong \frac{n}{2}K_2$. Otherwise $\Delta \geq 2$ then G contains a connected component H with atleast 3 vertices. If $H = K_n, n \geq 3$ then by lemma 2.6 $|\lambda_1^w| = 2(n-1)(n-2)$ and $|\lambda_2^w| = 2(n-2)$ clearly $|\lambda_1^w| > |\lambda_2^w|$ a contradiction. Otherwise H is not a complete graph then by Lemma 2.3 $\lambda_2^w \geq 0$ and from lemma 2.6 $\lambda_1^w > \lambda_2^w$ a contradiction. Conversely, one can easily check that $|\lambda_1^w| = |\lambda_2^w| = \dots = |\lambda_n^w|$ holds for $\overline{K_n}$ and $\frac{n}{2}K_2$.

3 Main Results

In this section, we obtained lower and upper bounds for spectral radius and energy of edge mass adjacency matrix of graphs.

Theorem 1. Let G be an n -vertex graph of size m with maximum degree Δ and minimum degree δ . Then

$$\lambda_1^w(G) \geq 4(\Delta - 1) \quad (17)$$

with equality holding if and only if G is a regular graph.

Proof: Let w_1, w_2, \dots, w_n be non-negative weights assigned to $v_i \in V(G)$ and $e_i \in E(G)$ with the condition that:

For $v_i \in V(G), w(v_i) = d_G(v_i)$ and for $e_i \in E(G), w(e) = d_G(u) + d_G(v) - 2$ where $e_i = uv$. Let $x = (x_1, x_2, \dots, x_n)^T$ be any unit vector in \mathbb{R}^n , then

$$\begin{aligned}
 x^T A^w(G)x &= \sum_{i=1}^n d_G^w(v_i)x_i x_j \\
 &= 2 \sum_{uv \in E(G)} [d_G(u) + d_G(v) - 2]x_i x_j \\
 &\geq 2(2(\Delta - 1)) \sum_{uv \in E(G)} x_i x_j \quad (18)
 \end{aligned}$$

putting $x = \left(\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}, \dots, \frac{1}{\sqrt{m}}\right)^T$ in (2) we get

$$x^T A^w(G)x \geq 4(\Delta - 1)$$

then by lemma 2.1 we have

$$\lambda_1^w \geq x^T A^w(G)x$$

combining this with the above result we get (17). The first part of the proof is done.

The equality in (18) holds if and only if $d_i = d_j = \delta = \Delta$, for each edge $v_i v_j \in E$, that is, G is regular.

Further, $A^w(G) = 2(\Delta - 1)A(G)$, $\lambda_1^w = 2(\Delta - 1)\lambda_1$. Since, $A(G)x = \Delta x$, $A^w(G)x = \lambda_1^w x$.

It follows that $x = \left(\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}, \dots, \frac{1}{\sqrt{m}}\right)^T$ is an eigenvalue λ_1^w . Hence the equality holds in (17) if and only if G is a regular graph.

Theorem 2. Let $G = (V, E)$ be a connected graph with $|V| = n$ and $|E| = m$ with maximum degree Δ . Then

$$\lambda_1^w \leq 2(\Delta - 1)\sqrt{2m - n + 1} \quad (19)$$

with equality if and only if $G \cong K_n, n \geq 2$.

Proof: Let λ_1^w be the spectral radius of the matrix $2(\Delta - 1)A(G)$ then by lemma 2.2 we get

$$\begin{aligned}
 \lambda_1^w &\leq 2(\Delta - 1)\lambda_1 \\
 &\leq 2(\Delta - 1)\sqrt{2m - n + 1}
 \end{aligned}$$

By lemma 2.4 it can be easily concluded that equality in (19) holds if and only if $G \cong K_n, n \geq 2$.

Theorem 3. If G is a connected graph with n vertices and λ_1^w is the spectral radius (the largest eigenvalue), then

$$\lambda_1^w \leq \sqrt{\frac{2(n-1)EM_1(G)}{n}} \quad (20)$$

Proof: Since $\sum_{i=1}^n \lambda_i^w = 0$ it can be rewritten as $\sum_{i=2}^n \lambda_i^w = -\lambda_1^w$. Further $(\sum_{i=1}^n (\lambda_i^w)^2) = 2EM_1(G)$, $(\sum_{i=2}^n (\lambda_i^w)^2) = (\sum_{i=1}^n (\lambda_i^w)^2) - (\lambda_1^w)^2 = (2EM_1(G) - (\lambda_1^w)^2)$ and $(\sum_{i=2}^n 1) = (n - 1)$.

Put $r_i = 1$ and $s_i = \lambda_i^w$ in lemma 2.6 we get

$$\begin{aligned} \left(\sum_{i=2}^n (\lambda_i^w)\right)^2 &\leq (n-1) \sum_{i=2}^n (\lambda_i^w)^2 \\ (-\lambda_1^w)^2 &\leq (n-1)(2EM_1(G) - (\lambda_1^w)^2) \\ (-\lambda_1^w)^2 &\leq (n-1)2EM_1(G) - (n-1)(\lambda_1^w)^2 \\ (-\lambda_1^w)^2 &\leq (n-1)2EM_1(G) - n(\lambda_1^w)^2 + (\lambda_1^w)^2 \\ n(\lambda_1^w)^2 &\leq (n-1)2EM_1(G) \\ \lambda_1^w &\leq \sqrt{\frac{2(n-1)EM_1(G)}{n}} \end{aligned}$$

Hence the proof.

Theorem 4. Let G be a connected graph with n vertices, then

$$\sqrt{2EM_1(G)} \leq E_w(G) \leq \sqrt{2nEM_1(G)} \tag{21}$$

Proof: For upper bound, consider the lemma 2.6 i.e.,

$$\left(\sum_{i=1}^n r_i s_i\right)^2 \leq \left(\sum_{i=1}^n r_i^2\right) \left(\sum_{i=1}^n s_i^2\right)$$

put $r_i = 1$ and $s_i = |\lambda_i^w|^2$ in lemma 2.6, we get

$$\left(\sum_{i=1}^n |\lambda_i^w|\right)^2 \leq \left(\sum_{i=1}^n 1^2\right) \left(\sum_{i=1}^n (|\lambda_i^w|^2)\right)$$

since $(\sum_{i=1}^n |\lambda_i^w|) = E_w(G)$, $(\sum_{i=1}^n 1^2) = n$ and $(\sum_{i=1}^n (|\lambda_i^w|^2)) = 2EM_1(G)$ we have

$$\begin{aligned} (E_w(G))^2 &\leq n \cdot 2EM_1(G) \\ E_w(G) &\leq \sqrt{2nEM_1(G)} \end{aligned}$$

Similarly, for lower bound consider the lemma 2.11 i.e.,

$$\left(\sum_{i=1}^n |r_i|\right)^2 \geq \left(\sum_{i=1}^n |r_i|^2\right)$$

put $r_i = |\lambda_i^w|$ in lemma 2.11 we get,

$$\begin{aligned} (E_w(G))^2 &\geq 2EM_1(G) \\ E_w(G) &\geq \sqrt{2EM_1(G)} \end{aligned}$$

Hence, combining upper bound and lower bound we get the required result.

Theorem 5. Let G be a graph with n vertices and m edges, then

$$E_w(G) \geq \sqrt{2nEM_1(G) - \frac{n^2}{4}(|\lambda_1^w| - |\lambda_n^w|)^2} \quad (22)$$

where $|\lambda_1^w|$ and $|\lambda_n^w|$ are maximum and minimum values of $|\lambda_i^w|$.

Proof: Let $|\lambda_1^w| \geq |\lambda_2^w| \geq \dots \geq |\lambda_n^w|$ be the eigenvalues of $A_w(G)$. By putting $r_i = 1$, $s_i = |\lambda_i^w|$, $p_1 = 1$, $p_2 = |\lambda_n^w|$ in lemma 2.8 we get

$$\sum_{i=1}^n (1)^2 \sum_{i=1}^n (|\lambda_i^w|^2) - \left[\sum_{i=1}^n |\lambda_i^w| \right]^2 \leq \frac{n^2}{4} (|\lambda_1^w| - |\lambda_n^w|)^2$$

since $(\sum_{i=1}^n |\lambda_i^w|^2) = 2EM_1(G)$ we have

$$\begin{aligned} 2nEM_1(G) - (E_w(G))^2 &\leq \frac{n^2}{4} (|\lambda_1^w| - |\lambda_n^w|)^2 \\ 2nEM_1(G) - \frac{n^2}{4} (|\lambda_1^w| - |\lambda_n^w|)^2 &\leq (E_w(G))^2 \\ E_w(G) &\geq \sqrt{2nEM_1(G) - \frac{n^2}{4} (|\lambda_1^w| - |\lambda_n^w|)^2} \end{aligned}$$

Hence the proof.

Theorem 6. Let G be a graph with n vertices and m edges. Let $\lambda_1^w \geq \lambda_2^w \geq \dots \geq \lambda_n^w$ be the eigenvalues of $A_w(G)$. Then

$$E_w(G) \geq \sqrt{2nEM_1(G) - \alpha(n)(|\lambda_1^w| - |\lambda_n^w|)^2} \quad (23)$$

where $\alpha(n) = n \left[\frac{n}{2} \right] \left(1 - \frac{1}{n} \left[\frac{n}{2} \right] \right)$.

Proof: Let $|\lambda_1^w| \geq |\lambda_2^w| \geq \dots \geq |\lambda_n^w|$ be the eigenvalues of $A_w(G)$. By putting $r_i = |\lambda_i^w| = s_i$, $R = |\lambda_1^w| = S$ and $r = |\lambda_n^w| = s$ in lemma 2.13 we get

$$\begin{aligned} \left| n \sum_{i=1}^n |\lambda_i^w|^2 - \left(\sum_{i=1}^n |\lambda_i^w| \right)^2 \right| &\leq \alpha(n) (|\lambda_1^w| - |\lambda_n^w|)^2 \\ |2nEM_1(G) - (E_w(G))^2| &\leq \alpha(n) (|\lambda_1^w| - |\lambda_n^w|)^2 \\ 2nEM_1(G) - \alpha(n) (|\lambda_1^w| - |\lambda_n^w|)^2 &\leq (E_w(G))^2 \\ E_w(G) &\geq \sqrt{2nEM_1(G) - \alpha(n) (|\lambda_1^w| - |\lambda_n^w|)^2} \end{aligned}$$

Hence the proof.

Theorem 7. If eigenvalues of $A_w(G)$ are non-zero. Then

$$E_w(G) \geq \frac{2\sqrt{|\lambda_1^w||\lambda_n^w|}\sqrt{2EM_1(G)}}{|\lambda_1^w| + |\lambda_n^w|} \quad (24)$$

where $|\lambda_1^w|$ and $|\lambda_n^w|$ are maximum and minimum of $|\lambda_i^w|$.

Proof: Let $|\lambda_1^w| \geq |\lambda_2^w| \geq \dots \geq |\lambda_n^w|$ be the eigenvalues of $A_w(G)$. By putting $r_i = |\lambda_i|$ and $s_i = 1$ in lemma 2.12 we get

$$\begin{aligned} \sum_{i=1}^n |\lambda_i^w|^2 \sum_{i=1}^n 1^2 &\leq \frac{1}{4} \left(\sqrt{\frac{|\lambda_1^w|}{|\lambda_n^w|}} + \sqrt{\frac{|\lambda_n^w|}{|\lambda_1^w|}} \right)^2 \left(\sum_{i=1}^n |\lambda_i^w| \right)^2 \\ 2nEM_1(G) &\leq \frac{1}{4} \left(\frac{(|\lambda_1^w| + |\lambda_n^w|)^2}{|\lambda_1^w| |\lambda_n^w|} \right) (E_w(G))^2 \\ \frac{2nEM_1(G) \cdot 4|\lambda_1^w| |\lambda_n^w|}{(|\lambda_1^w| + |\lambda_n^w|)^2} &\leq (E_w(G))^2 \\ E_w(G) &\geq \frac{2\sqrt{|\lambda_1^w| |\lambda_n^w|} \sqrt{2nEM_1(G)}}{|\lambda_1^w| + |\lambda_n^w|} \end{aligned}$$

Hence the proof.

Theorem 8. Let G be a graph with n vertices and m edges. Let $\lambda_1^w \geq \lambda_2^w \geq \dots \geq \lambda_n^w$ be the eigenvalues of $A_w(G)$. Then

$$E_w(G) \geq \frac{n + 2EM_1(G)(\lambda_n^w \lambda_1^w)}{\lambda_n^w + \lambda_1^w} \quad (25)$$

Proof: Let $\lambda_1^w \geq \lambda_2^w \geq \dots \geq \lambda_n^w$ be the eigenvalues of $A_w(G)$. By putting $r_i = |\lambda_i^w|$, $s_i = 1$, $p = \lambda_n^w$ and $P = \lambda_1^w$, in lemma 2.14 we get

$$\begin{aligned} \sum_{i=1}^n 1^2 + \lambda_n^w \lambda_1^w \sum_{i=1}^n |\lambda_i^w|^2 &\leq (\lambda_n^w + \lambda_1^w) \left(\sum_{i=1}^n |\lambda_i^w| \right) \\ n + 2EM_1(G)(\lambda_n^w \lambda_1^w) &\leq (\lambda_n^w + \lambda_1^w) E_w(G) \\ E_w(G) &\geq \frac{n + 2EM_1(G)(\lambda_n^w \lambda_1^w)}{\lambda_n^w + \lambda_1^w} \end{aligned}$$

Hence the proof.

Theorem 9. Let G be a graph with n vertices and m edges. Let $\lambda_1^w \geq \lambda_2^w \geq \dots \geq \lambda_n^w$ be the eigenvalues of $A_w(G)$. Then

$$E_w(G) \geq \frac{2EM_1(G) + n\lambda_1^w \lambda_n^w}{\lambda_1^w + \lambda_n^w} \quad (26)$$

Proof: Let $\lambda_1^w \geq \lambda_2^w \geq \dots \geq \lambda_n^w$ be the eigenvalues of $A_w(G)$. By putting $r_i = |\lambda_i^w|$, $s_i = 1$, $p = \lambda_n^w$ and $P = \lambda_1^w$, in lemma 2.14 we get

$$\begin{aligned} \sum_{i=1}^n |\lambda_i^w|^2 + \lambda_n^w \lambda_1^w \sum_{i=1}^n 1^2 &\leq (\lambda_n^w + \lambda_1^w) \left(\sum_{i=1}^n |\lambda_i^w| \right) \\ 2EM_1(G) + n(\lambda_n^w \lambda_1^w) &\leq (\lambda_n^w + \lambda_1^w) E_w(G) \\ E_w(G) &\geq \frac{2EM_1(G) + n\lambda_1^w \lambda_n^w}{\lambda_1^w + \lambda_n^w} \end{aligned}$$

Hence the proof.

Theorem 10. If G is a non-empty graph of order n . Then

$$E_w(G) \leq \sqrt{2(EM_1(G))^2 + \frac{n^2}{2}} \quad (27)$$

Proof: Let $\lambda_1^w \geq \lambda_2^w \geq \dots \geq \lambda_n^w$ be the eigenvalues of $A_w(G)$. Substituting $p_i = |\lambda_i^w| = q_i$ and $r_i = s_i = m_i = n_i = 1$ in lemma 2.9 we get

$$\begin{aligned} \sum_{i=1}^n 1 \cdot |\lambda_i^w|^2 \sum_{i=1}^n 1 \cdot |\lambda_i^w|^2 + \sum_{i=1}^n 1 \cdot 1^2 \sum_{i=1}^n 1 \cdot 1^2 &\geq 2 \sum_{i=1}^n 1 \cdot |\lambda_i^w| \cdot 1 \sum_{i=1}^n 1 \cdot |\lambda_i^w| \cdot 1 \\ 2EM_1(G) \cdot 2EM_1(G) + n \cdot n &\geq 2(E_w(G))^2 \\ 4(EM_1(G))^2 + n^2 &\geq 2(E_w(G))^2 \\ \sqrt{\frac{4(EM_1(G))^2 + n^2}{2}} &\geq E_w(G) \\ E_w(G) &\leq \sqrt{2(EM_1(G))^2 + \frac{n^2}{2}} \end{aligned}$$

4 Applications on edge mass energy of graphs

Until now many researchers have studied the predictive potential of molecular descriptors (mainly degree, distance and eigenvalue based) for predicting the π -electron energy of benzenoid hydrocarbons and also for measuring boiling point and enthalpy of formation of polycyclic aromatic compounds. In this section, we calculate energy and edge mass energy for molecular graphs of 22 benzenoid hydrocarbons which is listed in Table 1. The adjacency matrix is defined and eigenvalues, energy and edge mass energy are calculated using python programming language. The correlation, regression models are obtained for physiochemical properties of 22 benzenoid hydrocarbons, for which the data is taken from [17] (refer Table 2) and the predictive ability are tested using energy $E(G)$ and edge mass energy $E_w(G)$. In Table 3, the values of 11 molecular descriptors for 22 benzenoid hydrocarbons are listed which are from [17].

4.1 Data set

Table 1 Graph energy $E(G)$ and edge mass energy $E_w(G)$ of benzenoid hydrocarbons.

Benzenoid hydrocarbons	$E(G)$	$E_w(G)$
Naphthalene	13.684	33.92994
Phenanthrene	19.488	51.86194
Anthracene	19.3136	51.763186
Chrysene	25.192	69.74482
Tetraphene	25.104	87.365348

Triphenylene	25.276	71.69452
Naphthacene	27.3178	69.568754
Benzo[a]pyrene	28.2219	82.242794
Benzo[e]pyrene	28.3360	82.37146
Perylene	28.2453	82.208618
Anthanthrene	31.2528	94.986946
Benzo[ghi]perylene	31.4250	94.95264
Dibenz[a,h]anthracene	30.880	86.646292
Dibenz[a,j]anthracene	30.879	87.69062
Picene	30.942	87.64762
Coronene	34.568	107.64814
Benzo[c]phenanthrene	13.252	69.71874
Pyrene	22.505	64.405992
Dibenzo[a,e]pyrene	34.604	99.165458
Dibenzo[a,h]pyrene	33.926	100.048094
Dibenzo[a,i]pyrene	34.018	100.121532
Dibenzo[a,l]pyrene	34.030	100.135362

Table 2 Experimental values of some physiochemical properties of benzenoid hydrocarbons[17].

Benzenoid hydrocarbons	Boiling point(BP) (° C)	Entropy(S)	Acentric Factor (ω)	log P	Retention Index(RI)	Enthalpy ΔH_f
Naphthalene	218.000	79.38	0.302	3.30	200.00	150.6
Phenanthrene	338.000	93.79	0.394	4.46	300.00	209.1
Anthracene	340.050	92.43	0.402	4.45	301.69	218.3
Chrysene	431.000	106.83	0.460	5.81	400.00	267.7
Tetraphene	425.000	108.22	0.460	5.76	398.50	276.9
Triphenylene	429.000	104.66	0.460	5.49	400.00	258.5
Naphthacene	440.000	105.47	0.460	5.76	408.30	286.1
Benzo[a]pyrene	496.000	111.85	-	6.13	453.44	279.9

Benzo[e]pyrene	493.000	110.46	-	6.44	450.73	289.1
Perylene	497.000	109.10	0.490	6.25	456.22	279.9
Anthanthrene	547.000	114.10	-	7.04	503.89	310.5
Benzo[ghi]perylene	542.000	114.10	-	6.63	501.32	301.3
Dibenz[a,h]anthracene	536.000	119.87	-	6.75	495.45	335.5
Dibenz[a,j]anthracene	531.000	119.87	-	6.54	489.80	335.5
Picene	519.000	119.87	0.540	7.11	500.00	326.3
Coronene	590.000	116.36	0.540	7.64	549.67	322.7
Benzo[c]phenanthrene	448.000	113.61	-	5.70	391.12	280.5
Pyrene	404.000	96.06	0.410	4.88	351.22	230.5
Dibenzo[a,e]pyrene	592.000	124.89	-	7.28	551.53	338.5
Dibenzo[a,h]pyrene	596.000	123.50	-	7.28	559.90	347.7
Dibenzo[a,i]pyrene	594.000	123.50	-	7.28	556.47	347.7
Dibenzo[a,l]pyrene	595.000	131.69	-	7.71	553.00	351.2

Table 3 Molecular descriptors of benzenoid hydrocarbons[17].

Benzenoid hydrocarbons	M_1	M_2	F	R	ABC	SCI	GA	HA	SD	ReZ	RR
Naphthalene	50 .0 0	57 .0 0	11 8. 00	4.9 663 2	7.7 377 3	5.1 971 0	10. 919 18	4.9 333 3	22. 666 66	270. 0000 0	24. 797 95
Phenanthrene	76 .0 0	91 .0 0	18 8. 00	6.9 494 8	11. 192 38	7.4 080 2	15. 878 77	6.9 000 0	33. 000 00	454. 0000 0	37. 696 93
Anthracene	76 .0 0	90 .0 0	18 8. 00	6.9 326 5	11. 232 82	7.3 942 0	15. 838 36	6.8 666 6	33. 333 33	444. 0000 0	37. 595 91
Chrysene	10 2. 00	12 5. 00	25 8. 00	8.9 326 5	14. 647 04	9.6 189 5	20. 838 36	8.8 666 6	43. 333 33	638. 0000 0	50. 595 91

Tetraphene	10 2. 00	12 4. 00	25 8. 00	8.9 158 1	14. 687 48	9.6 051 2	20. 797 95	8.8 333 3	43. 666 66	628. 0000 0	50. 494 89
Triphenylene	10 2. 00	12 6. 00	25 8. 00	8.9 494 8	14. 606 60	9.6 327 7	20. 878 77	8.9 000 0	43. 000 00	648. 0000 0	50. 696 93
Naphthacene	10 2. 00	12 3. 00	25 8. 00	8.8 989 7	14. 727 92	9.5 913 0	20. 757 55	8.8 000 0	44. 000 00	618. 0000 0	50. 393 87
Benzo[a]pyrene	12 0. 00	15 1. 00	31 2. 00	9.9 158 1	16. 687 48	10. 829 87	23. 797 95	9.8 333 3	49. 666 66	790. 0000 0	59. 494 89
Benzo[e]pyrene	12 0. 00	15 2. 00	31 2. 00	9.9 326 5	16. 647 04	10. 843 69	23. 838 36	9.8 666 6	49. 333 33	800. 0000 0	59. 595 91
Perylene	12 0. 00	15 2. 00	31 2. 00	9.9 326 5	16. 647 04	10. 843 69	23. 838 36	9.8 666 6	49. 333 33	800. 0000 0	59. 595 91
Anthanthrene	13 8. 00	17 7. 00	36 6. 00	10. 898 97	18. 727 92	12. 040 79	26. 757 55	10. 800 00	56. 000 00	942. 0000 0	68. 393 87
Benzo[ghi]perylene	13 8. 00	17 8. 00	36 6. 00	10. 915 81	18. 687 48	12. 054 61	26. 797 95	10. 833 33	55. 666 66	952. 0000 0	68. 494 89
Dibenz[a,h]anthracene	12 8. 00	15 8. 00	32 8. 00	10. 898 97	18. 142 13	11. 816 05	25. 757 55	10. 800 00	54. 000 00	812. 0000 0	63. 393 87
Dibenz[a,j]anthracene	12 8. 00	15 8. 00	32 8. 00	10. 898 97	18. 142 13	11. 816 05	25. 757 55	10. 800 00	54. 000 00	812. 0000 0	63. 393 87
Picene	12 8. 00	15 9. 00	32 8. 00	10. 915 81	18. 101 69	11. 829 87	25. 797 95	10. 833 33	53. 666 66	822. 0000 0	63. 494 89
Coronene	15 6. 00	20 4. 00	42 0. 00	11. 898 97	20. 727 92	13. 265 54	29. 757 55	11. 800 00	62. 000 00	1104. 000 00	77. 393 87
Benzo[c]phenanthrene	10 2. 00	12 5. 00	25 8. 00	8.9 326 5	14. 647 04	9.6 189 5	20. 838 36	8.8 666 6	43. 333 33	638. 0000 0	50. 595 91

Pyrene	94 .0 0	11 7. 00	24 2. 00	7.9 326 5	13. 232 82	8.6 189 5	18. 838 36	7.8 666 6	39. 333 33	606. 0000 0	46. 595 91
Dibenzo[a,e]pyren e	14 6. 00	18 6. 00	38 2. 00	11. 915 81	20. 101 69	13. 054 61	28. 797 95	11. 833 33	59. 666 66	984. 0000 0	72. 494 89
Dibenzo[a,h]pyren e	14 6. 00	18 5. 00	38 2. 00	11. 898 97	20. 142 13	13. 040 79	28. 757 55	11. 800 00	60. 000 00	974. 0000 0	72. 393 89
Dibenzo[a,i]pyren e	14 6. 00	18 5. 00	38 2. 00	11. 898 97	20. 142 13	13. 040 79	28. 757 55	11. 800 00	60. 000 00	974. 0000 0	72. 393 89
Dibenzo[a,l]pyren e	14 6. 00	18 6. 00	38 2. 00	11. 915 81	20. 101 69	13. 054 61	28. 797 95	11. 933 33	59. 666 66	984. 0000 0	72. 494 89

5 Results and discussions

The intercorelation between physiochemical properties of benzenoid hydrocarbons such as boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient (log P), Kovats retention index(RI), and enthalpy of formation(ΔH_f) with graph energy $E(G)$ and edge mass energy $E_w(G)$ is analysed in Table 4. Also the intercorelation between 11 molecular descriptors such as first Zagreb index(M_1), second Zagreb index (M_2), F-index or forgotten index (F), Randić index (R), reciprocal Randić index(RR), atom bond connectivity index(ABC), sum division degree index(SDD), and redefined Zagreb index(ReZM) with graph energy $E(G)$ and edge mass energy $E_w(G)$ is listed in Table 5. We observe that the 11 molecular descriptors are highly intercorelated with edge mass energy $E_w(G)$ with $r > 0.97$ which is highlighted in Table 5.

Table 4 Corellation coefficient r between graph energy $E(G)$, edge mass energy $E_w(G)$ and physiochemical properties.

Energy	BP	S	ω	log P	RI	ΔH_f
$E(G)$	0.900	0.811	0.977	0.900	0.921	0.863
$E_w(G)$	0.969	0.913	0.937	0.969	0.974	0.930

Table 5 Corellation coefficient r between graph energy $E(G)$, edge mass energy $E_w(G)$ and molecular descriptors.

Degree based Molecular Descriptors	$E(G)$	$E_w(G)$
M_1	0.914	0.980

M_2	0.909	0.977
F	0.911	0.978
R	0.911	0.974
RR	0.915	0.979
ABC	0.914	0.977
SCI	0.914	0.979
GA	0.911	0.973
HA	0.916	0.979
SDD	0.903	0.972
ReZM	0.913	0.980

5.1 Regression models

The quadratic regression models for physiochemical properties (PP) such as boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient (log P), Kovats retention index (RI), and enthalpy of formation (ΔH_f) are derived with respect to graph energy $E(G)$ and edge mass energy $E_w(G)$. The symbols n, r, F are used to represent population, correlation coefficient, F-values.

The quadratic regression model is defined as

$$PP = a(E(G))^2 + b(E(G)) + c$$

The quadratic regression of PP with $E(G)$ are as follows:

$$BP = (-10.219)(E(G))^2 + (0.489)(E(G)) + (375.526)$$

$$n = 22 \quad r = 0.9230 \quad F = 54.872^\circ C$$

$$S = (-2.101)(E(G))^2 + (0.074)(E(G)) + (109.805)$$

$$n = 22 \quad r = 0.8491 \quad F = 24.597^\circ C$$

$$\omega = (0.020)(E(G))^2 + (0.000)(E(G)) + (0.067)$$

$$n = 22 \quad r = 0.9823 \quad F = 111.040^\circ C$$

$$\log P = (-0.123)(E(G))^2 + (0.006)(E(G)) + (4.986)$$

$$n = 22 \quad r = 0.9241 \quad F = 55.578^\circ C$$

$$RI = (-8.919)(E(G))^2 + (0.462)(E(G)) + (323.656)$$

$$n = 22 \quad r = 0.9428 \quad F = 75.994^\circ C$$

$$\Delta H_f = (-4.631)(E(G))^2 + (0.236)(E(G)) + (229.191)$$

$$n = 22 \quad r = 0.8831 \quad F = 33.780^\circ C$$

The quadratic regression of PP with $E_w(G)$ are as follows:

$$\begin{aligned}
 BP &= (7.026)(E_w(G))^2 + (-0.13)(E_w(G)) + (3.434) \\
 &\quad n = 22 \quad r = 0.9705 \quad F = 153.726^\circ C \\
 S &= (1.118)(E_w(G))^2 + (-0.004)(E_w(G)) + (44.689) \\
 &\quad n = 22 \quad r = 0.9208 \quad F = 52.889^\circ C \\
 \omega &= (0.007)(E_w(G))^2 + (-2.494)(E_w(G)) + (0.110) \\
 &\quad n = 22 \quad r = 0.9544 \quad F = 41.147^\circ C \\
 \log P &= (0.070)(E_w(G))^2 + (-6.907)(E_w(G)) + (1.030) \\
 &\quad n = 22 \quad r = 0.9695 \quad F = 149.803^\circ C \\
 RI &= (5.987)(E_w(G))^2 + (-0.007)(E_w(G)) + (6.350) \\
 &\quad n = 22 \quad r = 0.9741 \quad F = 175.069^\circ C \\
 \Delta H_f &= (4.853)(E_w(G))^2 + (-0.015)(E_w(G)) + (2.607) \\
 &\quad n = 22 \quad r = 0.9386 \quad F = 70.070^\circ C
 \end{aligned}$$

5.2 Analysis

The following analysis can be made from the quadratic regression models:

- The correlation coefficient r for quadratic regression models gives high predictability for physiochemical properties with respect to graph energy $E(G)$ and edge mass energy $E_w(G)$.
- The quadratic regression models for $E(G)$ gives high intercorelation with correlation coefficient $r = 0.9823$ for acentric factor.
- The quadratic regression model for $E(G)$ gives appreciable intercorelation with correlation coefficient $r = 0.9230$ for boiling point, $r = 0.9241$ for log P, $r = 0.9428$ for retention index.
- The quadratic regression model for $E(G)$ is weakly intercorelation with correlation coefficient $r = 0.8491$ for entropy and $r = 0.8831$ for enthalpy.
- The quadratic regression models for $E_w(G)$ gives high intercorelation with correlation coefficient $r = 0.9705$ for boiling point and $r = 0.9741$ for retention index.
- The quadratic regression model for $E_w(G)$ gives appreciable intercorelation with correlation coefficient $r = 0.9208$ for entropy, $r = 0.9544$ for acentfac, $r = 0.9695$ for log P and $r = 0.9386$ for enthalpy.

The scattered curve diagram of $E(G)$ with physiochemical properties are depicted in the following figures.

The scattered curve diagram of $E_w(G)$ with physiochemical properties are depicted in the following figures.

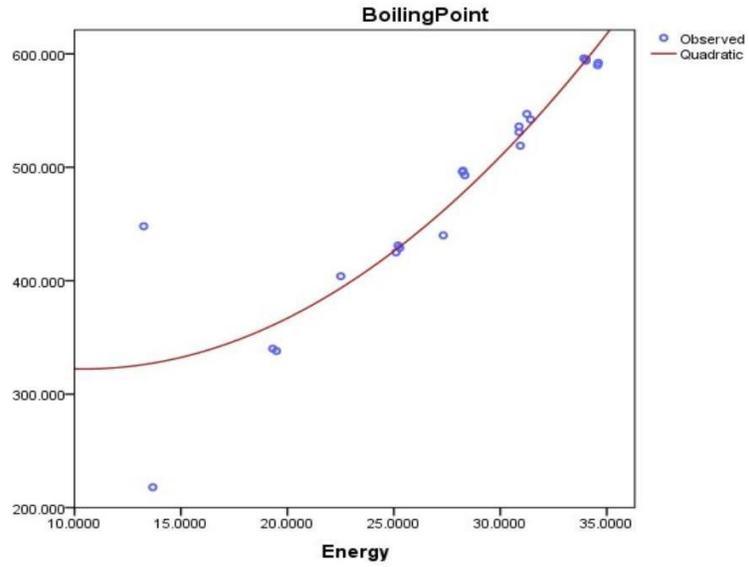


Fig. 1 The quadratic regression model for Boiling point with $E(G)$.

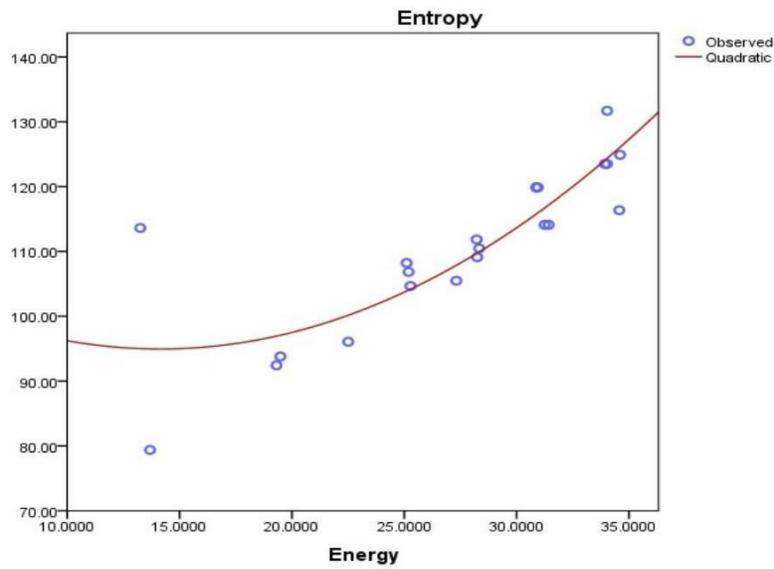


Fig. 2 The quadratic regression model for Entropy with $E(G)$.

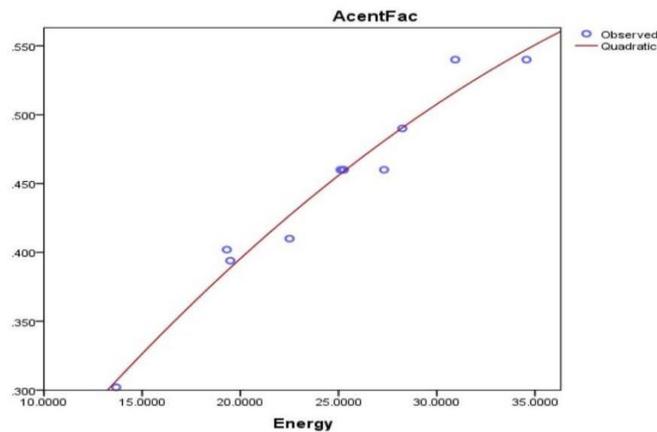


Fig. 3 The quadratic regression model for Acentric factor with $E(G)$.

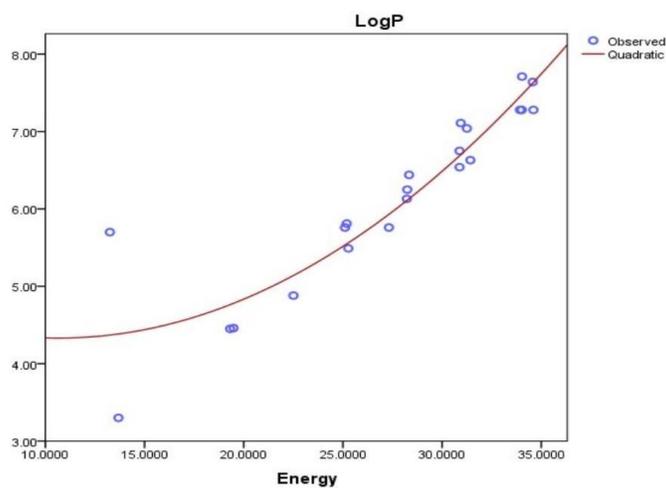


Fig. 4 The quadratic regression model for log P with $E(G)$.

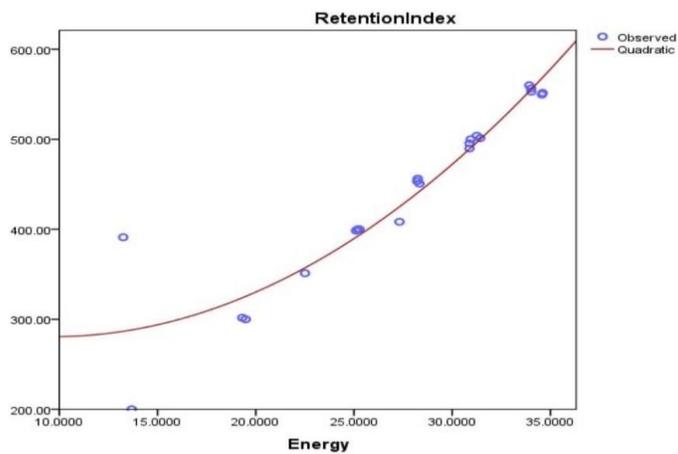


Fig. 5 The quadratic regression model for Retention index with $E(G)$.

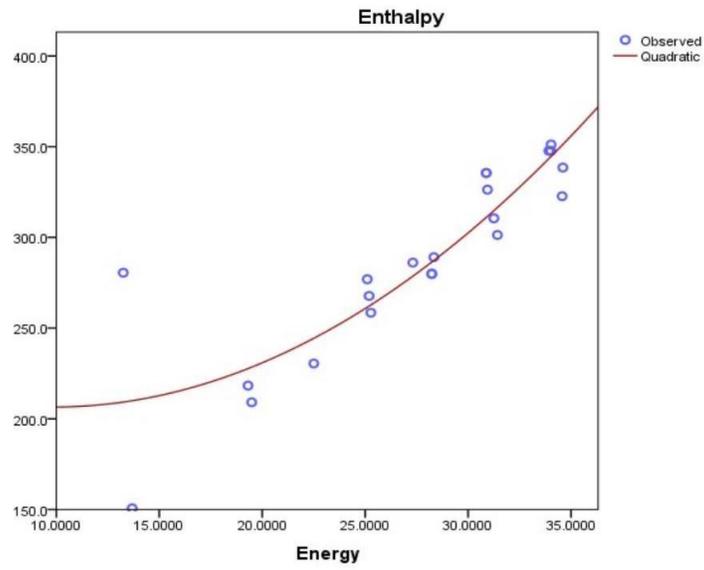


Fig. 6 The cubic regression model for Enthalpy with $E(G)$.

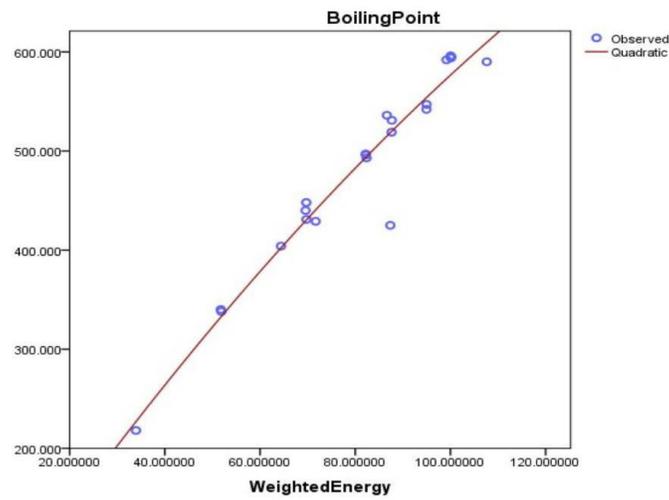


Fig. 7 The quadratic regression model for Boiling point with $E_w(G)$.

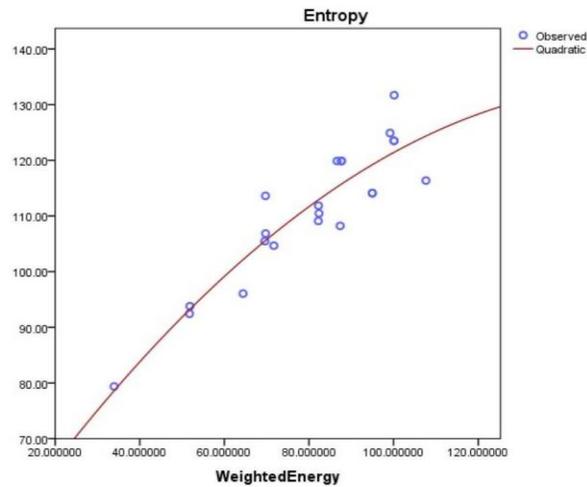


Fig. 8 The quadratic regression model for Entropy with $E_w(G)$.

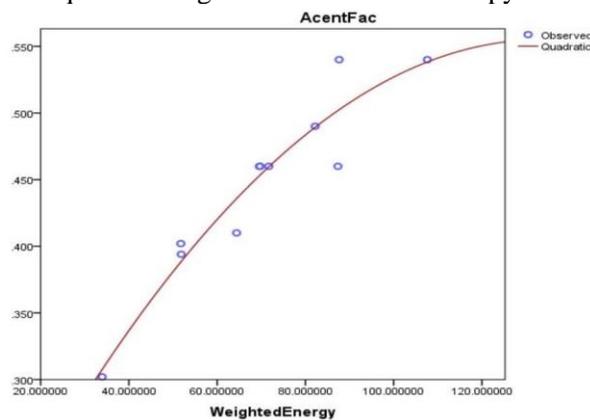


Fig. 9 The quadratic regression model for Acentric factor with $E_w(G)$.

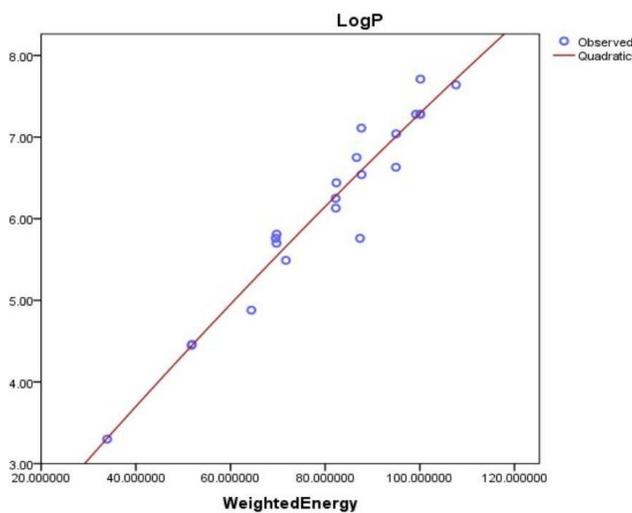


Fig. 10 The quadratic regression model for log P with $E_w(G)$.

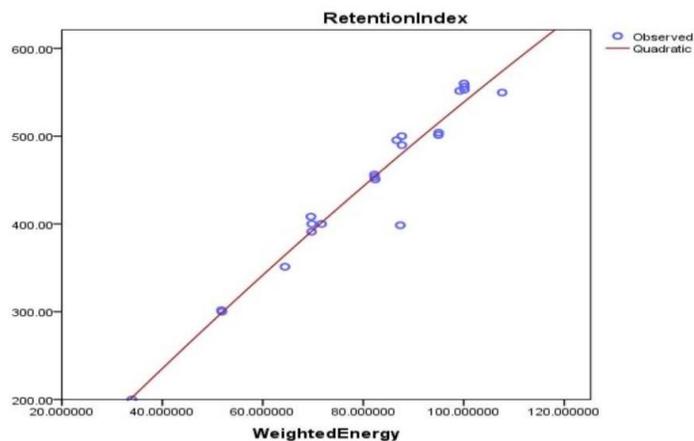


Fig. 11 The quadratic regression model for Retention index with $E_w(G)$.

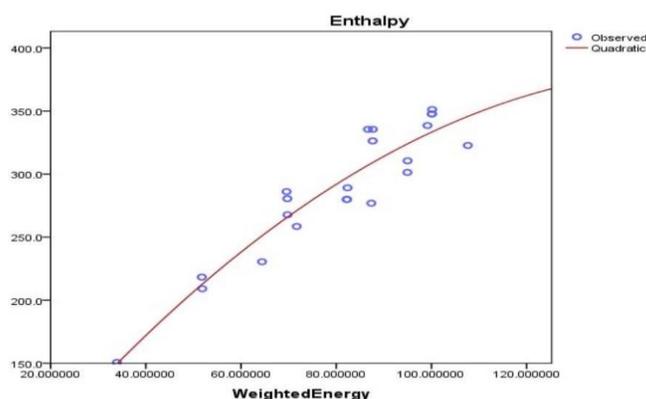


Fig. 12 The quadratic regression model for Enthalpy with $E_w(G)$.

Conclusion

In this paper, we define edge mass adjacency matrix $A_w(G)$ of a graph G such that, for any v_i that is adjacent to v_j , its (i, j) -entry equals $d_G(v_i) + d_G(v_j) - 2$; otherwise, it equals 0. The spectral radius λ_1^w and the energy $E_w(G)$ of the $A_w(G)$ are studied and lower and upper bounds are obtained for λ_1^w and $E_w(G)$. Further we calculated graph energy and edge mass energy of 22 benzenoid hydrocarbons by drawing its molecular graphs to check the predictive potential of physicochemical properties of benzenoid hydrocarbons. We derived quadratic regression models for boiling point (BP), entropy (S), acentric factor (ω), octanol-water partition coefficient ($\log P$), Kovats retention index (RI), and enthalpy of formation (ΔH_f) using these two graph energies. We also found correlation coefficient of physicochemical properties and molecular descriptors of benzenoid hydrocarbons with respect to graph energy $E(G)$ and edge mass energy $E_w(G)$.

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