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Research article

A novel edge-weighted matrix of a graph and its spectral properties with potential applications

Sakander Hayat[1,*], Sunilkumar M. Hosamani[2], Asad Khan[3,*], Ravishankar L. Hutagi[2], Umesh S. Mujumdar[2] and Mohammed J. F. Alenazi[4],

[1] Mathematical Sciences, Faculty of Science, Universiti Brunei Darussalam, Jln Tungku Link, Gadong BE1410, Brunei Darussalam

[2] Department of Mathematics, Rani Channamma University's Sangolli Rayanna First Grade Constituent College, Belagavi, 590001, India

[3] Metaverse Research Institute, School of Computer Science and Cyber Engineering, Guangzhou University, Guangzhou, Guangdong 510006, China

[4] Department of Computer Engineering, College of Computer and Information Sciences (CCIS), King Saud University, Riyadh 11451, Saudi Arabia

* **Correspondence:** Email: sakander1566@gmail.com (S.H.), asad@gzhu.edu.cn (A.K.); Tel: +673-8632409.

Abstract: Regarding a simple graph Γ possessing ν vertices (ν-vertex graph) and m edges, the vertex-weight and weight of an edge $e = uv$ are defined as $w(v_i) = d_\Gamma(v_i)$ and $w(e) = d_\Gamma(u) + d_\Gamma(v) - 2$, where $d_\Gamma(v)$ is the degree of v. This paper puts forward a novel graphical matrix named the edge-weighted adjacency matrix (adjacency of the vertices) $A_w(\Gamma)$ of a graph Γ and is defined in such a way that, for any v_i that is adjacent to v_j, its (i, j)-entry equals $w(e) = d_\Gamma(v_i) + d_\Gamma(v_j) - 2$; otherwise, it equals 0. The eigenvalues $\lambda_1^w \geq \lambda_2^w \geq \ldots \geq \lambda_\nu^w$ of A_w are called the edge-weighted eigenvalues of Γ. We investigate the mathematical properties of $A_w(\Gamma)$'s spectral radius λ_1^w and energy $E_w(\Gamma) = \sum_{i=1}^{\nu} |\lambda_i^w|$. Sharp lower and upper bounds are obtained for λ_1^w and $E_w(\Gamma)$, and the respective extremal graphs are characterized. Further, we employ these spectral descriptors in structure-property modeling of the physicochemical properties of polycyclic aromatic hydrocarbons for a set of benzenoid hydrocarbons (BHs). Detailed regression analysis showcases that edge-weighted energy outperforms classical adjacency energy in structure-property modeling of the physicochemical properties of BHs.

Keywords: edge weight energy; spectral radius; benzenoid hydrocarbons; structure-property modeling; graphical descriptor
Mathematics Subject Classification: 05C12, 05C50, 05C92

1. Introduction

Every graph taken into consideration here is a simple graph $\Gamma = (V, E)$, where $|V| = \nu$ and $|E| = m$. The count of edges connected to a vertex $v \in V$, denoted by $d_\Gamma(v)$ is the degree of that vertex. The degree of an edge $e = uv$ is defined by $d_\Gamma(e) = d_\Gamma(u) + d_\Gamma(v) - 2$. The parameters Δ (resp. δ) and $\Delta'(\delta')$ represent the maximum (resp. minimum) vertex and edge degree of a graph, respectively. If $\Delta_\Gamma = \delta_\Gamma = \nu - 1$ then the graph Γ is said to be a complete graph denoted by K_ν. The graph Γ is called bipartite if $V(\Gamma)$ is partitioned into two sets say, M and N (partite sets), such that every edge in Γ has one endpoint in M and the other in N. If every vertex of M is adjacent to every vertex of N with $|M| = r$ and $|N| = s$, then the graph is called the complete bipartite graph, denoted as $K_{r,s}$. The graph $K_{1,\nu-1}$ denoted by S_ν is a star graph, and the graph $K_{r,r}$ is called the equi-bipartite graph. The graph $\overline{\Gamma}$ represents the complement of a graph Γ, which is defined on the same vertex set as Γ such that if two vertices are adjacent in $\overline{\Gamma}$, then they are not adjacent in Γ. For more graph-theoretic terminologies, we refer to the book by Harary [19]. For any real number x, the floor function is the greatest integer less than or equal to x, denoted as $\lfloor x \rfloor$.

The first degree-based molecular descriptor, the Zagreb index, was developed by Gutman and Trinajstić [9]. It first emerged in the topological formula for conjugated molecules regarding their total π-electron energy. The first Zagreb index is defined as:

$$M_1(\Gamma) = \sum_{v \in V(\Gamma)} d_\Gamma(v)^2 = \sum_{e=uv \in E(\Gamma)} (d_\Gamma(u) + d_\Gamma(v)). \tag{1.1}$$

The Zagreb indices were reformulated in 2004 by Milićević et al. [28] in terms of edge degree, where the edge degree is given by $d_\Gamma(e) = d_\Gamma(u) + d_\Gamma(v) - 2$ for $e = uv \in E(\Gamma)$. Thus, the first reformulated Zagreb index is given by

$$EM_1(\Gamma) = \sum_{e \in E(\Gamma)} d_\Gamma(e)^2. \tag{1.2}$$

The reader is referred to [9] regarding applications of Zagreb indices.

The sum of the absolute values of eigenvalues of the adjacency matrix of Γ gives us the energy $E(\Gamma)$ of a graph Γ. This quantity is introduced in [10]. Suppose $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_\nu$ are the eigenvalues of the adjacency matrix $A(\Gamma)$, then the energy of the graph Γ is given by

$$E(\Gamma) = \sum_{i=1}^{\nu} |\lambda_i|. \tag{1.3}$$

Other graph energies were also introduced and studied. Indulal et al. [20] presented some results on the distance energy of graphs. Gutman and Zhou [8] investigated the Laplcaian energy of graphs and derived some extremal results from it.

The extended adjacency matrix of graph Γ was proposed by Yang et al. [36] in 1994, denoted by $A_{ex}(\Gamma)$. Its (i, j)-entry is defined to be 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 ν, all its eigenvalues are real, which are denoted as $\eta_1 \geq \eta_2 \geq \ldots \geq \eta_\nu$. Yang et al. [36] also investigated the extended graph energy by summing the absolute values of the eigenvalues of the A_{ex}-matrix, defined as

$$E_{ex}(\Gamma) = \sum_{i=1}^{\nu} |\eta_i|. \tag{1.4}$$

For recent studies on graph energy, we refer to [5, 6, 23, 24, 33, 35].

1.1. Edge-weighted graph energy

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

Definition 1.1. *Let $V = \{v_1, v_2, \ldots, v_\nu\}$ be the vertex set and $\{w_1, w_2, \ldots, w_\nu\}$ be the vertex-weights, then the vertex weight for $v_i \in V$ is defined as $w(v_i) = d_\Gamma(v_i)$. The range for a vertex-weight of $v_i \in V$ is $0 \leq w(v_i) \leq \Delta_\Gamma$ (here $w(v_i) = 0$ if Γ is disconnected).*

Definition 1.2. *Let $E_\Gamma = \{e_1, e_2, \ldots, e_m\}$ be the edge set, then the edge-weight of $e_i = u_i v_i$ is defined by $w(e_i) = d_\Gamma(u_i) + d_\Gamma(v_i) - 2$. The range for an edge-weight of $e \in E$ is $0 \leq w(e) \leq \frac{M_1(\Gamma)}{2} - m$ (where $w(e) = 0$ if and only if $\Gamma = K_2$.*

Definition 1.3. *The weighted degree of a vertex $v \in V(\Gamma)$ is defined as*

$$d_\Gamma^w(v) = \sum_{e=uv} w(e).$$

It is very clear that $w(e) = d_\Gamma(e)$ for every $e \in E$.

Observe that

$$\sum_{i=1}^{\nu} d_\Gamma^w(v_i) = 2\sum_{i=1}^{m} w(e_i) = 2\sum_{uv\in E}[d_\Gamma(u) + d_\Gamma(v) - 2] = 2[M_1 - 2m].$$

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

$$E_w = E_w(\Gamma) = \sum_{i=1}^{\nu} |\lambda_i^w|. \tag{1.5}$$

Following the types of adjacencies in [34], the type of adjacency employed by the edge-weighted matrix is the vertex-based adjacency.

1.2. Some useful identities

This subsection presents some basic properties of edge-weighted eigenvalues of graphs.

(1) $\sum_{i=1}^{\nu} \lambda_i^w = 0$.
(2) $\sum_{i=1}^{\nu} \left(\lambda_i^w\right)^2 = 2\sum_{i=1}^{m}[w(e_i)]^2 = 2\sum_{i=1}^{m} d_\Gamma(e_i)^2 = 2EM_1(\Gamma)$.
(3) $\sum_{0\leq i\leq j} \lambda_i^w \lambda_j^w = -\sum_{i=1}^{m}[w(e_i)]^2 = -\sum_{i=1}^{m} d_\Gamma(e_i)^2 = -EM_1(\Gamma)$.

Moreover, observe that,

(1) $\sum_{i=1}^{\nu} . \left(\lambda_i^w\right)^2 = 2EM_1(\Gamma)$.

(2) $\sum_{0\le i\le j}\lambda_i^w\lambda_j^w = -EM_1(\Gamma)$.

The following example delivers the edge-weighted energy of standard graph families.

Example 1.4. *(1) The edge-weighted energy $E_w(K_\nu)$ of K_ν is $4(\nu-1)(\nu-2)$.*
(2) The edge-weighted energy $E_w(K_{r,s})$ of $K_{r,s}$ is $2(r+s-2)\sqrt{rs}$.
(3) The edge-weighted energy $E_w(S_\nu)$ of S_ν is $2(\nu-2)\sqrt{(\nu-1)}$.
(4) The edge-weighted energy $E_w(K_{r,r})$ of $K_{r,r}$ is $4r(r-1)$.

Proof. The edge-weighted energy $E_w(K_{r,s})$ of $K_{r,s}$ is $2(r+s-2)\sqrt{rs}$. Replacing s by r in $E_w(K_{r,s})$ of $K_{r,s}$, we get $E_w(K_{r,r})$ of $K_{r,r}$ as $2(r+r-2)\sqrt{r^2} = 4r(r-1)$. □

2. Auxiliary results

In subsequent sections, we need the following already established results:

Lemma 2.1. *[35] Let $C = (c_{ij})$ and $D = (d_{ij})$ be real symmetric non-negative matrices of order ν. If $C \ge D$, i.e., $c_{ij} \ge d_{ij}$ for all i, j, then $\lambda_1(C) \ge \lambda_1(D)$, whereas λ_1 is the largest eigenvalue.*

Lemma 2.2. *[35] Let Γ be a connected graph of order ν with m edges. Then*

$$\lambda_1(\Gamma) \le \sqrt{2m-\nu+1} \tag{2.1}$$

with equality if and only if $\Gamma \cong K_{1,\nu-1}$ or $\Gamma \cong K_\nu$.

Here we deliver the well-known Cauchy–Schwartz inequality.

Lemma 2.3. *(Cauchy–Schwartz inequality) [3] Let r_i and s_i, $1 \le i \le \nu$ be any real numbers, then*

$$\left(\sum_{i=1}^{\nu} r_i s_i\right)^2 \le \left(\sum_{i=1}^{\nu} r_i^2\right)\left(\sum_{i=1}^{\nu} s_i^2\right). \tag{2.2}$$

The Ozeki inequality is frequently used in the spectral analysis of graphs.

Lemma 2.4. *(Ozeki inequality) [30] If r_i and s_i $(1 \le i \le \nu)$ are non-negative real numbers, then*

$$\sum_{i=1}^{\nu} r_i^2 \sum_{i=1}^{\nu} s_i^2 - \left[\sum_{i=1}^{\nu} r_i s_i\right]^2 \le \frac{\nu^2}{4}(P_1P_2 - p_1p_2)^2 \tag{2.3}$$

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

The following inequality has been retrieved from Dragomir [7].

Lemma 2.5. *[7] Let p_i, q_i, r_i and s_i be sequences of real numbers, and m_i, ν_i are non-negative for $i = 1, 2, \ldots, \nu$. Then the following inequality is valid:*

$$\sum_{i=1}^{\nu} m_i p_i^2 \sum_{i=1}^{\nu} \nu_i q_i^2 + \sum_{i=1}^{\nu} m_i r_i^2 \sum_{i=1}^{\nu} m_i s_i^2 \ge 2\sum_{i=1}^{\nu} m_i p_i r_i \sum_{i=1}^{\nu} \nu_i q_i s_i. \tag{2.4}$$

Jog and Gurjar [23] used the following inequality while studying bounds on the distance energy of graphs:

Lemma 2.6. *Let r_i, $1 \leq i \leq \nu$ be any real numbers, then*

$$\left(\sum_{i=1}^{\nu} |r_i|\right)^2 \geq \left(\sum_{i=1}^{\nu} |r_i|^2\right). \tag{2.5}$$

The following inequality was shown by Pólya and Szegó in their book [31].

Lemma 2.7. *[31] Suppose r_i and s_i, $1 \leq i \leq \nu$ are positive real numbers, then*

$$\sum_{i=1}^{\nu} r_i^2 \sum_{i=1}^{\nu} s_i^2 \leq \frac{1}{4}\left(\sqrt{\frac{P_1P_2}{p_1p_2}} + \sqrt{\frac{p_1p_2}{P_1P_2}}\right)^2 \left(\sum_{i=1}^{\nu} r_i s_i\right)^2 \tag{2.6}$$

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

The following classical inequality was proven by Biernacki et al. [2].

Lemma 2.8. *[2] Suppose r_i and s_i, $1 \leq i \leq \nu$ are positive real numbers, then*

$$|\nu \sum_{i=1}^{\nu} r_i s_i - \sum_{i=1}^{\nu} r_i \sum_{i=1}^{\nu} s_i| \leq \alpha(\nu)(R - r)(S - s) \tag{2.7}$$

where r, s, R, and S are real constants such that for each i, $1 \leq i \leq \nu$, $r \leq r_i \leq R$, and $s \leq s_i \leq S$. Further, $\alpha(\nu) = \nu\lfloor\frac{\nu}{2}\rfloor\left(1 - \frac{1}{\nu}\lfloor\frac{\nu}{2}\rfloor\right)$.

Diaz and Metcalf [4] delivered a proof of the following inequality:

Lemma 2.9. *[4] Let r_i and s_i, $1 \leq i \leq \nu$ are nonnegative real numbers, then*

$$\sum_{i=1}^{\nu} s_i^2 + pP \sum_{i=1}^{\nu} r_i^2 \leq (p + P)\left(\sum_{i=1}^{\nu} r_i s_i\right) \tag{2.8}$$

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

Next, we prove the following inequality on the edge-connected eigenvalues:

Lemma 2.10. *Let Γ be a connected graph of order $\nu \geq 2$. Then $\lambda_1^w > \lambda_2^w$.*

Proof. Let us assume, for the sake of contradiction, that $\lambda_1^w = \lambda_2^w$. Since Γ is connected, $A_w(\Gamma)$ is an irreducible non-negative $\nu \times \nu$ matrix. By the Perron–Frobenius theorem, the eigenvector 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. This implies that it would be possible to construct an eigenvector with some zero components, which contradicts the fact that all components of x are positive. Hence, we must have $\lambda_1^w > \lambda_2^w$. □

Next, we deliver a characterization for an ν-vertex satisfying $|\lambda_1^w| = |\lambda_2^w| = \ldots = |\lambda_\nu^w|$.

Proposition 2.11. *Let Γ be a graph of order ν. Then $|\lambda_1^w| = |\lambda_2^w| = \ldots = |\lambda_\nu^w|$ if and only if $\Gamma \cong \overline{K_\nu}$ or $\Gamma \cong \frac{\nu}{2}K_2$.*

Proof. First, assume that $|\lambda_1^w| = |\lambda_2^w| = \ldots = |\lambda_\nu^w|$. Let S be the number of isolated vertices in Γ. If $S \geq 1$, then $\lambda_1^w = \lambda_2^w = \ldots = \lambda_\nu^w = 0$, hence $\Gamma \cong \overline{K_\nu}$ or $\Gamma \cong \frac{\nu}{2}K_2$. Otherwise, if the maximum degree $\Delta \geq 2$, then Γ contains a connected component H with at least 3 vertices. If $H = K_\nu$, $\nu \geq 3$, then by Lemma 2.10, $|\lambda_1^w| = 2(\nu-1)(\nu-2)$ and $|\lambda_2^w| = 2(\nu-2)$, clearly $|\lambda_1^w| > |\lambda_2^w|$, a contradiction. Otherwise, if H is not a complete graph, then by Lemma 2.10, $\lambda_1^w > \lambda_2^w$, a contradiction.

Conversely, one can easily check that $|\lambda_1^w| = |\lambda_2^w| = \ldots = |\lambda_\nu^w|$ holds for $\overline{K_\nu}$ and $\frac{\nu}{2}K_2$. □

3. Main results

This section delivers various upper/lower extremal values for $E_w(\Gamma)$ and λ_1^w for an (m, ν)-graph with ν-vertices and m-edges.

A sharp upper bound on λ_1^w (i.e., edge-weighted spectral radius) is being proven in the following result.

Theorem 3.1. *Let Γ be an (m, ν)-graph possessing the maximum degree Δ. Then*

$$\lambda_1^w \leq 2\,(\Delta - 1)\,\sqrt{1 - \nu + 2m} \tag{3.1}$$

with $\lambda_1^w = 2\,(\Delta - 1)\,\sqrt{1 - \nu + 2m} \iff \Gamma \cong K_\nu$, $\nu \geq 2$.

Proof. Since $A_w(\Gamma) \leq 2(\Delta - 1)A(\Gamma)$ and λ_1^w be its spectral radius. Employing Lemma 2.1, one has

$$\lambda_1^w \leq 2\lambda_1(\Delta - 1).$$

By Lemma 2.2, one obtains

$$\lambda_1^w \leq 2(\Delta - 1)\sqrt{1 - \nu + 2m}.$$

Also, $\lambda_1^w = 2\,(\Delta - 1)\,\sqrt{1 - \nu + 2m}$ in (3.1) $\iff \Gamma \cong K_\nu$, $\nu \geq 2$. □

The next theorem delivers an upper extremal value considering the first–formulated Zagreb EM_1 index of Γ.

Theorem 3.2. *If Γ is an ν-vertex graph having λ_1^w as its spectral radius (the largest eigenvalue), then*

$$\lambda_1^w \leq \sqrt{\frac{2(-1+\nu)EM_1(\Gamma)}{\nu}}. \tag{3.2}$$

Proof. Since $\sum_{k=1}^{\nu} \lambda_k^w = 0$ it can be rewritten as $\sum_{k=2}^{\nu} \lambda_k^w = -\lambda_1^w$. Further, $\left(\sum_{k=1}^{\nu}(\lambda_k^w)^2\right) = 2EM_1(\Gamma)$, $(\sum_{k=2}^{\nu}(\lambda_k^w)^2) = (\sum_{k=1}^{\nu}(\lambda_k^w)^2 - (\lambda_1^w)^2) = (2EM_1(\Gamma) - (\lambda_1^w)^2)$ and $(\sum_{k=2}^{\nu} 1) = (\nu - 1)$.

Put $r_k = 1$ and $s_k = \lambda_k^w$ in Lemma 2.3 and we obtain

$$\begin{aligned} \left(\sum_{k=2}^{\nu}(\lambda_k^w)\right)^2 &\leq (\nu-1)\sum_{k=2}^{\nu}(\lambda_k^w)^2 \\ (-\lambda_1^w)^2 &\leq (-1+\nu)(2EM_1(\Gamma) - (\lambda_1^w)^2) \end{aligned}$$

$$\begin{aligned}(-\lambda_1^w)^2 &\leq (-1+\nu)2EM_1(\Gamma) - (\nu-1)(\lambda_1^w)^2\\ (-\lambda_1^w)^2 &\leq (-1+\nu)2EM_1(\Gamma) - \nu(\lambda_1^w)^2 + (\lambda_1^w)^2\\ \nu(\lambda_1^w)^2 &\leq (-1+\nu)2EM_1(\Gamma)\\ \lambda_1^w &\leq \sqrt{\frac{2(-1+\nu)EM_1(\Gamma)}{\nu}}.\end{aligned}$$

Hence, we have furnished the proof. □

Some lower and upper extremal values on E_w i.e., edge-weighted energy of Γ.

Theorem 3.3. *For a connected ν-vertex graph Γ, E_w satisfies*

$$\sqrt{2EM_1(\Gamma)} \leq E_w(\Gamma) \leq \sqrt{2\nu EM_1(\Gamma)}. \tag{3.3}$$

Proof. For the upper bound, consider Lemma 2.3, i.e.,

$$\left(\sum_{k=1}^{\nu} r_k s_k\right)^2 \leq \left(\sum_{k=1}^{\nu} r_k^2\right)\left(\sum_{k=1}^{\nu} s_k^2\right)$$

put $r_k = 1$ and $s_k = |\lambda_k^w|^2$ in Lemma 2.3, we obtain

$$\left(\sum_{k=1}^{\nu} |\lambda_k^w|\right)^2 \leq \left(\sum_{k=1}^{\nu} 1^2\right)\left(\sum_{k=1}^{\nu} (|\lambda_k^w|)^2\right)$$

since $\left(\sum_{k=1}^{\nu} |\lambda_k^w|\right) = E_w(\Gamma)$, $\left(\sum_{k=1}^{\nu} 1^2\right) = 1$ and $\left(\sum_{k=1}^{\nu} (|\lambda_k^w|)^2\right) = 2EM_1(\Gamma)$, we have

$$\begin{aligned}(E_w(\Gamma))^2 &\leq \nu \cdot 2EM_1(\Gamma)\\ E_w(\Gamma) &\leq \sqrt{2\nu EM_1(\Gamma)}.\end{aligned}$$

Similarly, for a lower bound, consider Lemma 2.6, i.e.,

$$\left(\sum_{k=1}^{\nu} |r_k|\right)^2 \geq \left(\sum_{k=1}^{\nu} |r_k|^2\right)$$

put $r_k = |\lambda_k^w|$ in Lemma 2.6, we obtan

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

Hence, by combining the upper bound and the lower bound, we obtain the required result. □

In terms of the EM_1 index, our next result delivers another lower extremal value on E_w.

Theorem 3.4. *Any (m, ν)-graph Γ satisfies*

$$E_w(\Gamma) \geq \sqrt{2\nu EM_1(\Gamma) - \frac{\nu^2}{4}(|\lambda_1^w| - |\lambda_\nu^w|)^2} \tag{3.4}$$

where $|\lambda_\nu^w|$ (resp. $|\lambda_1^w|$) are minimum (resp. maximum) values of $|\lambda_k^w|$.

Proof. Let $|\lambda_1^w| \geq |\lambda_2^w| \geq \ldots \geq |\lambda_\nu^w|$ be the eigenvalues of $A_w(\Gamma)$. By putting $r_k = 1$, $s_k = |\lambda_k^w|$ $P_1 = 1$, $P_2 = |\lambda_1^w|$, $p_1 = 1$ and $p_2 = |\lambda_\nu^w|$ in Lemma 2.4, one gets

$$\sum_{k=1}^{\nu}(1)^2 \sum_{k=1}^{\nu}(|\lambda_k^w|^2) - \left[\sum_{k=1}^{\nu}|\lambda_k^w|\right]^2 \leq \frac{\nu^2}{4}(|\lambda_1^w| - |\lambda_\nu^w|)^2$$

since $\left(\sum_{k=1}^{\nu}(\lambda_k^w)^2\right) = 2EM_1(\Gamma)$ we have

$$\begin{aligned} 2\nu EM_1(\Gamma) - (E_w(\Gamma))^2 &\leq \frac{\nu^2}{4}(|\lambda_1^w| - |\lambda_\nu^w|)^2 \\ 2\nu EM_1(\Gamma) - \frac{\nu^2}{4}(|\lambda_1^w| - |\lambda_\nu^w|)^2 &\leq (E_w(\Gamma))^2 \\ E_w(\Gamma) &\geq \sqrt{2\nu EM_1(\Gamma) - \frac{\nu^2}{4}(|\lambda_1^w| - |\lambda_\nu^w|)^2}. \end{aligned}$$

Hence, the proof has been furnished. □

The following theorem further refines the bound in Theorem 3.4.

Theorem 3.5. *For an (ν, m)-graph Γ, assume $\lambda_1^w \geq \lambda_2^w \geq \ldots \geq \lambda_\nu^w$ are eigenvalues of $A_w(\Gamma)$. This implies that,*

$$E_w(\Gamma) \geq \sqrt{2\nu EM_1(\Gamma) - \alpha(\nu)(|\lambda_1^w| - |\lambda_\nu^w|)^2} \tag{3.5}$$

where $\alpha(\nu) = \nu\lfloor\frac{\nu}{2}\rfloor\left(1 - \frac{1}{\nu}\lfloor\frac{\nu}{2}\rfloor\right)$.

Proof. Let $|\lambda_1^w| \geq |\lambda_2^w| \geq \ldots \geq |\lambda_\nu^w|$ be the eigenvalues of $A_w(\Gamma)$. By putting $r_k = |\lambda_k^w| = s_k$, $R = |\lambda_1^w| = S$, and $r = |\lambda_\nu^w| = s$ in Lemma 2.8, one obtains

$$\begin{aligned} |\nu\sum_{k=1}^{\nu}|\lambda_k^w|^2 - (\sum_{k=1}^{\nu}|\lambda_k^w|)^2| &\leq \alpha(\nu)(|\lambda_1^w| - |\lambda_\nu^w|)^2 \\ |2\nu EM_1(\Gamma) - (E_w(\Gamma))^2| &\leq \alpha(\nu)(|\lambda_1^w| - |\lambda_\nu^w|)^2 \\ 2\nu EM_1(\Gamma) - \alpha(\nu)(|\lambda_1^w| - |\lambda_\nu^w|)^2 &\leq (E_w(\Gamma))^2 \\ E_w(\Gamma) &\geq \sqrt{2\nu EM_1(\Gamma) - \alpha(\nu)(|\lambda_1^w| - |\lambda_\nu^w|)^2}. \end{aligned}$$

Hence the proof has been furnished. □

For a non-zero eigenvalue of a graph, the following theorem delivers yet another lower bound on the edge-weighted energy E_w of graphs.

Theorem 3.6. *If the eigenvalues of $A_w(\Gamma)$ are non-zero, then*

$$E_w(\Gamma) \geq \frac{2\sqrt{|\lambda_1^w||\lambda_\nu^w|}\sqrt{2EM_1(\Gamma)}}{|\lambda_1^w| + |\lambda_\nu^w|}, \tag{3.6}$$

where $|\lambda_1^w|$ and $|\lambda_\nu^w|$ are the maximum and minimum of $|\lambda_k^w|$.

Proof. Let $|\lambda_1^w| \geq |\lambda_2^w| \geq \ldots \geq |\lambda_\nu^w|$ be the eigenvalues of $A_w(\Gamma)$. By putting $r_k = |\lambda_k|$ and $s_k = 1$ in Lemma 2.7, we obtain

$$\begin{aligned}
\sum_{k=1}^{\nu} |\lambda_k^w|^2 \sum_{k=1}^{\nu} 1^2 &\leq \frac{1}{4}\left(\sqrt{\frac{|\lambda_1^w|}{|\lambda_\nu^w|}} + \sqrt{\frac{|\lambda_\nu^w|}{|\lambda_1^w|}}\right)^2 \left(\sum_{k=1}^{\nu} |\lambda_k^w|\right)^2 \\
2\nu EM_1(\Gamma) &\leq \frac{1}{4}\left(\frac{(|\lambda_1^w| + |\lambda_2^w|)^2}{|\lambda_1^w||\lambda_\nu^w|}\right)(E_w(\Gamma))^2 \\
\frac{2\nu EM_1(\Gamma) \cdot 4|\lambda_1^w||\lambda_\nu^w|}{(|\lambda_1^w| + |\lambda_\nu^w|)^2} &\leq (E_w(\Gamma))^2 \\
E_w(\Gamma) &\geq \frac{2\sqrt{|\lambda_1^w||\lambda_\nu^w|}\sqrt{2\nu EM_1(\Gamma)}}{|\lambda_1^w| + |\lambda_\nu^w|}.
\end{aligned}$$

Hence the proof is completed. □

The following two results deliver lower bounds on E_w in terms of EM_1, the smallest and largest eigenvalues of graphs.

Theorem 3.7. *Assuming $\lambda_1^w \geq \lambda_2^w \geq \ldots \geq \lambda_\nu^w$ to be the eigenvalues of $A_w(\Gamma)$, where Γ is an (ν, m)-graph. Then*

$$E_w(\Gamma) \geq \frac{\nu + 2EM_1(\Gamma)(\lambda_\nu^w \lambda_1^w)}{\lambda_\nu^w + \lambda_1^w}. \tag{3.7}$$

Proof. Let $\lambda_1^w \geq \lambda_2^w \geq \ldots \geq \lambda_\nu^w$ be the eigenvalues of $A_w(\Gamma)$. By putting $r_k = |\lambda_k^w|$, $s_k = 1$, $p = \lambda_\nu^w$ and $P = \lambda_1^w$, in Lemma 2.9, we obtain

$$\begin{aligned}
\sum_{k=1}^{\nu} 1^2 + \lambda_\nu^w \lambda_1^w \sum_{k=1}^{\nu} |\lambda_k^w|^2 &\leq (\lambda_\nu^w + \lambda_1^w)\left(\sum_{k=1}^{\nu} |\lambda_k^w|\right) \\
\nu + 2EM_1(\Gamma)(\lambda_\nu^w \lambda_1^w) &\leq (\lambda_\nu^w + \lambda_1^w)E_w(\Gamma) \\
E_w(\Gamma) &\geq \frac{\nu + 2EM_1(\Gamma)(\lambda_\nu^w \lambda_1^w)}{\lambda_\nu^w + \lambda_1^w}.
\end{aligned}$$

Hence, the proof has been completed. □

Theorem 3.8. *Assuming $\lambda_1^w \geq \lambda_2^w \geq \ldots \geq \lambda_\nu^w$ to be the eigenvalues of $A_w(\Gamma)$, where Γ is an (ν, m)-graph, then*

$$E_w(\Gamma) \geq \frac{2EM_1(\Gamma) + \nu\lambda_1^w \lambda_\nu^w}{\lambda_1^w + \lambda_\nu^w}. \tag{3.8}$$

Proof. Let $\lambda_1^w \geq \lambda_2^w \geq \ldots \geq \lambda_\nu^w$ be the eigenvalues of $A_w(\Gamma)$. By putting $r_k = |\lambda_k^w|$, $s_k = 1$, $p = \lambda_\nu^w$ and $P = \lambda_1^w$, in Lemma 2.9, we obtain

$$\begin{aligned}
\sum_{k=1}^{\nu} |\lambda_k^w|^2 + \lambda_\nu^w \lambda_1^w \sum_{k=1}^{\nu} 1^2 &\leq (\lambda_\nu^w + \lambda_1^w)\left(\sum_{k=1}^{\nu} |\lambda_k^w|\right) \\
2EM_1(\Gamma) + \nu(\lambda_\nu^w \lambda_1^w) &\leq (\lambda_\nu^w + \lambda_1^w)E_w(\Gamma) \\
E_w(\Gamma) &\geq \frac{2EM_1(\Gamma) + \nu\lambda_1^w \lambda_\nu^w}{\lambda_1^w + \lambda_\nu^w}.
\end{aligned}$$

Hence the proof has been furnished. □

Next, a sharp upper extremal value on E_w is proven.

Theorem 3.9. *If Γ is a non-empty graph of order ν. Then*

$$E_w(\Gamma) \leq \sqrt{2(EM_1(\Gamma))^2 + \frac{\nu^2}{2}}. \tag{3.9}$$

Proof. Let $\lambda_1^w \geq \lambda_2^w \geq \ldots \geq \lambda_\nu^w$ be the eigenvalues of $A_w(\Gamma)$. Substituting $p_k = |\lambda_k^w| = q_k$ and $r_k = s_k = m_k = \nu_k = 1$ in Lemma 2.5, we obtain

$$\begin{aligned}
\sum_{k=1}^{\nu} 1 \cdot |\lambda_k^w|^2 \sum_{k=1}^{\nu} 1 \cdot |\lambda_k^w|^2 + \sum_{k=1}^{\nu} 1 \cdot 1^2 \sum_{k=1}^{\nu} 1 \cdot 1^2 &\geq 2 \sum_{k=1}^{\nu} 1 \cdot |\lambda_k^w| \cdot 1 \sum_{k=1}^{\nu} 1 \cdot |\lambda_k^w| \cdot 1 \\
2EM_1(\Gamma) \cdot 2EM_1(\Gamma) + \nu \cdot \nu &\geq 2(E_w(\Gamma))^2 \\
4(EM_1(\Gamma))^2 + \nu^2 &\geq 2(E_w(\Gamma))^2 \\
\sqrt{\frac{4(EM_1(\Gamma))^2 + \nu^2}{2}} &\geq E_w(\Gamma) \\
E_w(\Gamma) &\leq \sqrt{2(EM_1(\Gamma))^2 + \frac{\nu^2}{2}}.
\end{aligned}$$

□

4. Applications on the edge-weighted energy of graphs

Until now, many researchers have studied the predictive potential of molecular descriptors (mainly degree-, distance-, and eigenvalue-based) for estimating the π-electron energy (E_π) of benzenoid hydrocarbons (BHs) and also for estimating the enthalpy of formation ΔH_f^o and boiling point B_p of BHs. For instance, Hayat et al. [16] (resp. Hayat and coauthors [14, 27]) investigated the efficiency of degree-dependent (resp. eigenvalues-dependent) graphical descriptors for estimating E_π of BHs. Similar studies were conducted by Hayat et al. [15] (Hayat and Liu [12]) for distance-related and temperature-based graphical descriptors. For predicting physicochemical properties such as B_p and ΔH_f^o of BHs, comparative studies for distance-dependent, temperature-related, degree-related, and eigenvalue-related descriptors were conducted in [13, 17, 18, 26], respectively. For more studies on QSPR, we refer to [1, 11, 29, 32].

In this section, we calculate energy and edge-weighted energy for molecular graphs of 22 benzenoid hydrocarbons which are listed in Table 1. The adjacency matrix is defined, and eigenvalues, energy, and edge-weighted energy are calculated using the Python programming language. The correlation and regression models are obtained for the physicochemical properties of 22 BHs, for which the data is taken from [25] (refer to Table 2), and the predictive ability is tested using energy $E(\Gamma)$ and edge-weighted energy $E_w(\Gamma)$. In Table 3, the values of 11 molecular descriptors for 22 BHs are listed, which are from [25]. Note that we consider carbon–carbon structures as chemical graphs. One can consider other construction, of chemical graph based on molecular alignment [22].

This subsection records all the data sets that we employ for our structure-property models.

Table 1. Edge-weighted energy $E_w(\Gamma)$ and graph energy $E(\Gamma)$ of lower 22 BHs.

Compound	$E_w(\Gamma)$	$E(\Gamma)$
Naphthalene	33.92994	13.684
Anthracene	51.763186	19.3136
Phenanthrene	51.86194	19.488
Pyrene	64.405992	22.505
Naphthacene	69.568754	27.3178
Triphenylene	71.69452	25.276
Tetraphene	87.365348	25.104
Benzo[c]phenanthrene	69.71874	13.252
Chrysene	69.74482	25.192
Perylene	82.208618	28.2453
Benzo[e]pyrene	82.37146	28.3360
Benzo[a]pyrene	82.242794	28.2219
Benzo[ghi]perylene	94.95264	31.4250
Anthanthrene	94.986946	31.2528
Picene	87.64762	30.942
Dibenz[a,j]anthracene	87.69062	30.879
Dibenz[a,h]anthracene	86.646292	30.880
Dibenzo[a,l]pyrene	100.135362	34.030
Dibenzo[a,i]pyrene	100.121532	34.018
Dibenzo[a,h]pyrene	100.048094	33.926
Dibenzo[a,e]pyrene	99.165458	34.604
Coronene	107.64814	34.568

Table 2. Experimental data on certain physicochemical characteristics of BHs [25].

Compound	Boiling point (BP)(°C)	Entropy(S) (Cal/mol.K)	Acentric Factor (ω)	log P	Retention Index (RI)	Enthalpy ΔH_f^o (kJ/mol)
Naphthalene	218.000	79.38	0.302	3.30	200.00	150.6
Anthracene	340.050	92.43	0.402	4.45	301.69	218.3
Phenanthrene	338.000	93.79	0.394	4.46	300.00	209.1
Pyrene	404.000	96.06	0.410	4.88	351.22	230.5
Naphthacene	440.000	105.47	0.460	5.76	408.30	286.1
Triphenylene	429.000	104.66	0.460	5.49	400.00	258.5
Tetraphene	425.000	108.22	0.460	5.76	398.50	276.9
Benzo[c]phenanthrene	448.000	113.61	-	5.70	391.12	280.5
Chrysene	431.000	106.83	0.460	5.81	400.00	267.7
Perylene	497.000	109.10	0.490	6.25	456.22	279.9
Benzo[e]pyrene	493.000	110.46	-	6.44	450.73	289.1
Benzo[a]pyrene	496.000	111.85	-	6.13	453.44	279.9
Benzo[ghi]perylene	542.000	114.10	-	6.63	501.32	301.3
Anthanthrene	547.000	114.10	-	7.04	503.89	310.5
Picene	519.000	119.87	0.540	7.11	500.00	326.3
Dibenz[a,j]anthracene	531.000	119.87	-	6.54	489.80	335.5
Dibenz[a,h]anthracene	536.000	119.87	-	6.75	495.45	335.5
Dibenzo[a,l]pyrene	595.000	131.69	-	7.71	553.00	351.2
Dibenzo[a,i]pyrene	594.000	123.50	-	7.28	556.47	347.7
Dibenzo[a,h]pyrene	596.000	123.50	-	7.28	559.90	347.7
Dibenzo[a,e]pyrene	592.000	124.89	-	7.28	551.53	338.5
Coronene	590.000	116.36	0.540	7.64	549.67	322.7

Table 3. Molecular graphical descriptors of the lower 22 BHs [25].

Compound	M_1	M_2	F	R	ABC	SCI
Naphthalene	50.00	57.00	118.00	4.96632	7.73773	5.19710
Anthracene	76.00	90.00	188.00	6.93265	11.23282	7.39420
e Phenanthrene	76.00	91.00	188.00	6.94948	11.19238	7.40802
Pyrene	94.00	117.00	242.00	7.93265	13.23282	8.61895
Naphthacene	102.00	123.00	258.00	8.89897	14.72792	9.59130
Triphenylene	102.00	126.00	258.00	8.94948	14.60660	9.63277
Tetraphene	102.00	124.00	258.00	8.91581	14.68748	9.60512
Benzo[c]phenanthrene	102.00	125.00	258.00	8.93265	14.64704	9.61895
Chrysene	102.00	125.00	258.00	8.93265	14.64704	9.61895
Perylene	120.00	152.00	312.00	9.93265	16.64704	10.84369
Benzo[e]pyrene	120.00	152.00	312.00	9.93265	16.64704	10.84369
Benzo[a]pyrene	120.00	151.00	312.00	9.91581	16.68748	10.82987
Benzo[ghi]perylene	138.00	178.00	366.00	10.91581	18.68748	12.05461
Anthanthrene	138.00	177.00	366.00	10.89897	18.72792	12.04079
Picene	128.00	159.00	328.00	10.91581	18.10169	11.82987
Dibenz[a,j]anthracene	128.00	158.00	328.00	10.89897	18.14213	11.81605
Dibenz[a,h]anthracene	128.00	158.00	328.00	10.89897	18.14213	11.81605
Dibenzo[a,l]pyrene	146.00	186.00	382.00	11.91581	20.10169	13.05461
Dibenzo[a,i]pyrene	146.00	185.00	382.00	11.89897	20.14213	13.04079
Dibenzo[a,h]pyrene	146.00	185.00	382.00	11.89897	20.14213	13.04079
Dibenzo[a,e]pyrene	146.00	186.00	382.00	11.91581	20.10169	13.05461
Coronene	156.00	204.00	420.00	11.89897	20.72792	13.26554
Compound	**GA**	**HA**	**SDD**	**ReZM**	**RR**	-
Naphthalene	10.91918	4.93333	22.66666	270.00000	24.79795	
Anthracene	15.83836	6.86666	33.33333	444.00000	37.59591	
Phenanthrene	15.87877	6.90000	33.00000	454.00000	37.69693	
Pyrene	18.83836	7.86666	39.33333	606.00000	46.59591	
Naphthacene	20.75755	8.80000	44.00000	618.00000	50.39387	
Triphenylene	20.87877	8.90000	43.00000	648.00000	50.69693	
Tetraphene	20.79795	8.83333	43.66666	628.00000	50.49489	
Benzo[c]phenanthrene	20.83836	8.86666	43.33333	638.00000	50.59591	
Chrysene	20.83836	8.86666	43.33333	638.00000	50.59591	
Perylene	23.83836	9.86666	49.33333	800.00000	59.59591	
Benzo[e]pyrene	23.83836	9.86666	49.33333	800.00000	59.59591	
Benzo[a]pyrene	23.79795	9.83333	49.66666	790.00000	59.49489	
Benzo[ghi]perylene	26.79795	10.83333	55.66666	952.00000	68.49489	
Anthanthrene	26.75755	10.80000	56.00000	942.00000	68.39387	
Picene	25.79795	10.83333	53.66666	822.00000	63.49489	
Dibenz[a,j]anthracene	25.75755	10.80000	54.00000	812.00000	63.39387	
Dibenz[a,h]anthracene	25.75755	10.80000	54.00000	812.00000	63.39387	
Dibenzo[a,l]pyrene	28.79795	11.93333	59.66666	984.00000	72.49489	
Dibenzo[a,i]pyrene	28.75755	11.80000	60.00000	974.00000	72.39389	
Dibenzo[a,h]pyrene	28.75755	11.80000	60.00000	974.00000	72.39389	
Dibenzo[a,e]pyrene	28.79795	11.83333	59.66666	984.00000	72.49489	
Coronene	29.75755	11.80000	62.00000	1104.00000	77.39387	

5. Results and discussions

The intercorrelation between the physicochemical properties of polycyclic aromatic hydrocarbons, such as Kovats retention index (RI), acentric factor (ω), octanol-water partition coefficient ($\log P$), boiling point (BP), enthalpy of formation (ΔH_f) and entropy (S), with graph energy $E(\Gamma)$ and edge-weighted energy $E_w(\Gamma)$, is analysed in Table 4. Also, the intercorrelation between 11 molecular

descriptors such as atom bond connectivity index (ABC), forgotten index (F), 1st and 2nd Zagreb invariants (M_1 and M_2), sum division degree index (SDD), reciprocal Randić index (RR), classical Randić index (R), redefined Zagreb index (ReZM) with graph energy $E(\Gamma)$ and edge-weighted energy $E_w(\Gamma)$ is listed in Table 5. We observe that the 11 molecular descriptors are highly intercorrelated with edge-weighted energy $E_w(\Gamma)$ with r > 0.97, which is highlighted in Table 5.

Table 4. Correlation coefficient r between graph energy $E(\Gamma)$, edge-weighted energy $E_w(\Gamma)$, and physicochemical properties.

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

Table 5. Correlation coefficient r between graph energy $E(\Gamma)$, edge-weighted energy $E_w(\Gamma)$, and molecular descriptors.

Degree based Molecular Descriptors	$E(\Gamma)$	$E_w(\Gamma)$
M_1	0.914	0.980
M_2	0.909	0.977
ABC	0.914	0.977
ReZM	0.913	0.980
R	0.911	0.974
F	0.911	0.978
HA	0.916	0.979
SCI	0.914	0.979
RR	0.915	0.979
SDD	0.903	0.972
GA	0.911	0.973

The value of r for $E_w(\Gamma)$ ranges from 0.972 to 0.980.

5.1. Regression models

The quadratic regression models for physico-chemical properties (PPs) such as Kovats retention index (RI), acentric factor (ω), octanol–water partition coefficient (log P), boiling point (BP), enthalpy of formation (ΔH_f), and entropy (S) are derived with respect to graph energy $E(\Gamma)$ and edge-weighted energy $E_w(\Gamma)$. The symbols ν, r, F, and SE are used to represent population, correlation coefficient, F-values, and the standard error of the estimate, respectively. Note that, in general, quadratic models have very bad predictive power, even if they have good estimating power. The reader is referred to [21] for diversity in detailed regression analysis.

The quadratic regression model is defined as

$$PP = a(E(\Gamma))^2 + b(E(\Gamma)) + c.$$

The quadratic regression of PP with $E(\Gamma)$ is as follows:

$$BP = (0.489)(E(\Gamma))^2 + (-10.219)(E(\Gamma)) + (375.526).$$

$$\nu = 22 \quad \text{r} = 0.9230 \quad F = 54.872^{\circ}\text{C} \quad SE = 39.940.$$

$$S = (0.074)(E(\Gamma))^2 + (-2.101)(E(\Gamma)) + (109.805).$$

$$\nu = 22 \quad \text{r} = 0.8491 \quad F = 24.597^{\circ}\text{C} \quad SE = 6.838.$$

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

$$\nu = 22 \quad \text{r} = 0.9823 \quad F = 111.040^{\circ}\text{C} \quad SE = 0.014.$$

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

$$\nu = 22 \quad \text{r} = 0.9241 \quad F = 55.578^{\circ}\text{C} \quad SE = 0.460.$$

$$RI = (0.462)(E(\Gamma))^2 + (-8.919)(E(\Gamma)) + (323.656).$$

$$\nu = 22 \quad \text{r} = 0.9428 \quad F = 75.994^{\circ}\text{C} \quad SE = 33.759.$$

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

$$\nu = 22 \quad \text{r} = 0.8831 \quad F = 33.780^{\circ}\text{C} \quad SE = 25.526.$$

The quadratic regression of PP with $E_w(\Gamma)$ is as follows:

$$BP = (-0.013)(E_w(\Gamma))^2 + (7.026)(E_w(\Gamma)) + (3.434).$$

$$\nu = 22 \quad \text{r} = 0.9705 \quad F = 153.726^{\circ}\text{C} \quad SE = 25.082.$$

$$S = (-0.004)(E_w(\Gamma))^2 + (1.118)(E_w(\Gamma)) + (44.689).$$

$$\nu = 22 \quad \text{r} = 0.9208 \quad F = 52.889^{\circ}\text{C} \quad SE = 5.055.$$

$$\omega = (-2.494)(E_w(\Gamma))^2 + (0.007)(E_w(\Gamma)) + (0.110).$$

$$\nu = 22 \quad \text{r} = 0.9544 \quad F = 41.147^{\circ}\text{C} \quad SE = 0.023.$$

$$log\ P = (-6.907)(E_w(\Gamma))^2 + (0.070)(E_w(\Gamma)) + (1.030).$$

$$\nu = 22 \quad \text{r} = 0.9695 \quad F = 149.803^{\circ}\text{C} \quad SE = 0.294.$$

$$RI = (-0.007)(E_w(\Gamma))^2 + (5.987)(E_w(\Gamma)) + (6.350).$$

$$\nu = 22 \quad \text{r} = 0.9741 \quad F = 175.069^{\circ}\text{C} \quad SE = 22.976.$$

$$\Delta H_f = (-0.015)(E_w(\Gamma))^2 + (4.853)(E_w(\Gamma)) + (2.607).$$

$$\nu = 22 \quad \text{r} = 0.9386 \quad F = 70.070^{\circ}\text{C} \quad SE = 18.826.$$

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 physicochemical properties with respect to graph energy $E(\Gamma)$ and edge-weighted energy $E_w(\Gamma)$.
- The quadratic regression models for $E(\Gamma)$ give high intercorrelation with a correlation value of r = 0.9823 for the acentric factor.

- The degree-2 polynomial regression model for $E(\Gamma)$ gives appreciable intercorrelation with a correlation value of r = 0.9230 for the boiling point, r = 0.9241 for the log P, r = 0.9428 for the retention index.
- The quadratic regression model for $E(\Gamma)$ is weakly intercorrelation with correlation value r = 0.8491 for the entropy, and r = 0.8831 for the enthalpy.
- The quadratic regression models for $E_w(\Gamma)$ give high intercorrelation with a correlation value of r = 0.9705 for the boiling point and r = 0.9741 for retention index.
- The quadratic regression model for $E_w(\Gamma)$ gives appreciable intercorrelation with a correlation value of r = 0.9208 for entropy, r = 0.9544 for acentfac, r = 0.9695 for log P, and r = 0.9386 for the enthalpy.
- From all the 12 quadratic regression models, it has been observed that the significance F is 0.000.

The scattered curve diagram of $E(\Gamma)$ with physiochemical properties are depicted in Figures 1–6.

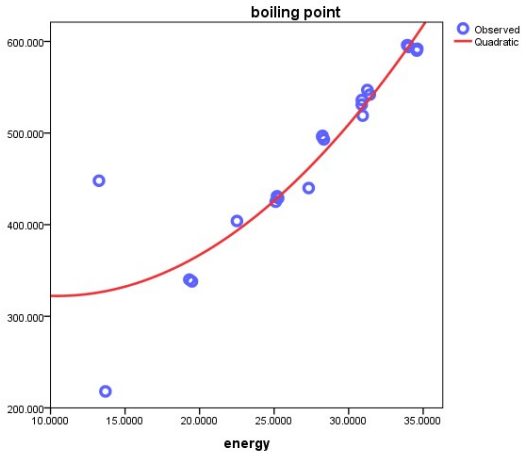

Figure 1. The quadratic regression model for boiling point with $E(\Gamma)$.

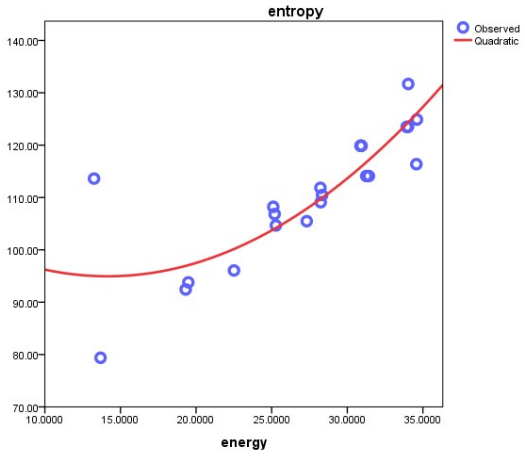

Figure 2. The quadratic regression model for entropy with $E(\Gamma)$.

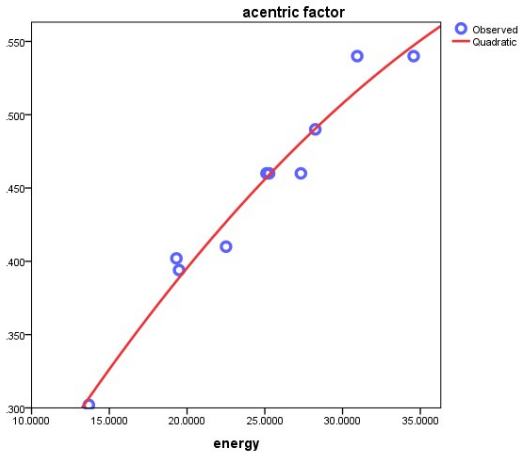

Figure 3. The quadratic regression model for acentric factor with $E(\Gamma)$.

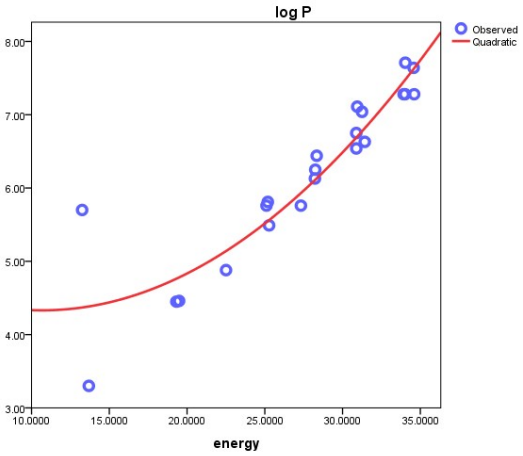

Figure 4. The quadratic regression model for log P with $E(\Gamma)$.

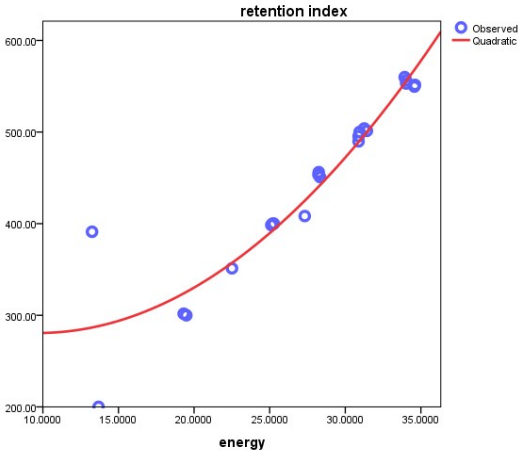

Figure 5. The quadratic regression model for retention index with $E(\Gamma)$.

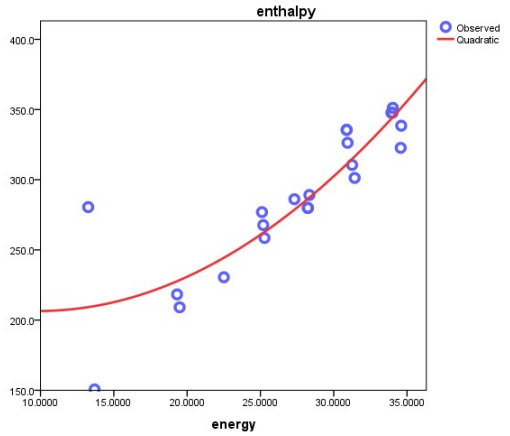

Figure 6. The quadratic regression model for enthalpy with $E(\Gamma)$.

The scattered curve diagram of $E_w(\Gamma)$ with physicochemical characteristics are depicted in Figures 7–12.

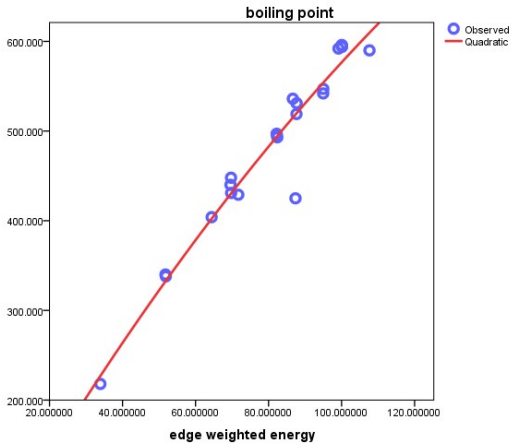

Figure 7. The quadratic regression model for boiling point with $E_w(\Gamma)$.

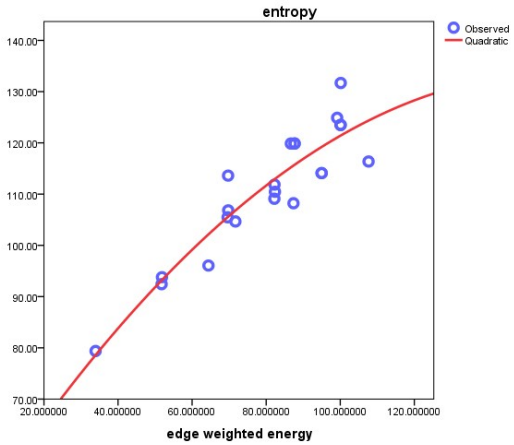

Figure 8. The quadratic regression model for entropy with $E_w(\Gamma)$.

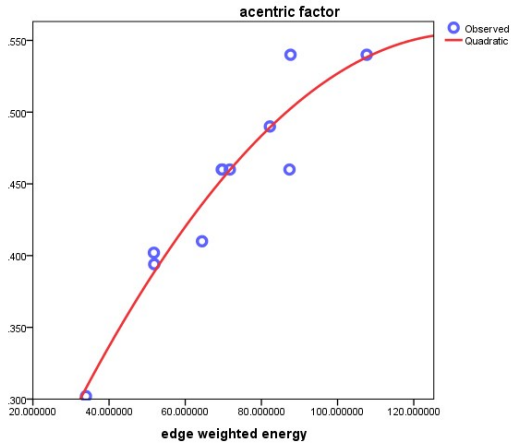

Figure 9. The quadratic regression model for acentric factor with $E_w(\Gamma)$.

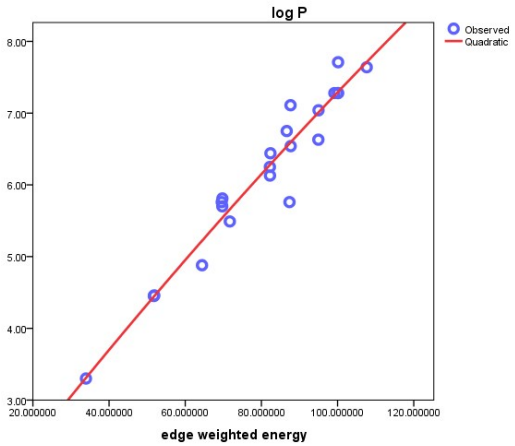

Figure 10. The quadratic regression model for log P with $E_w(\Gamma)$.

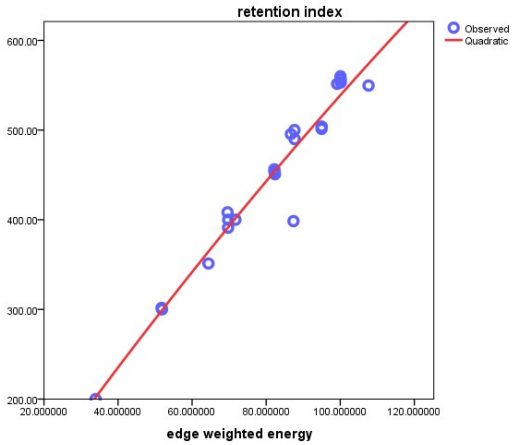

Figure 11. The quadratic regression model for retention index with $E_w(\Gamma)$.

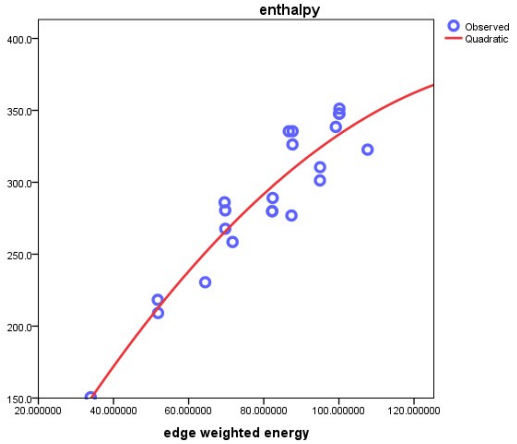

Figure 12. The quadratic regression model for enthalpy with $E_w(\Gamma)$.

6. Conclusions

This paper puts forward the edge-weighted adjacency matrix $A_w(\Gamma)$ of a graphical structure Γ. The energy $E_w(\Gamma)$ as well as the spectral radius λ_1^w of the $A_w(\Gamma)$ have been studied, and lower and upper extremes are derived for λ_1^w and $E_w(\Gamma)$ in terms of other graphical parameters. Further, we calculated the graph energy and edge-weighted energy of 22 BHs by drawing their molecular graphs to check the predictive potential of the physicochemical characteristics of BHs. Polynomials of degree-2 regression models were generated for Kovats retention index (RI), acentric factor (ω), octanol-water partition coefficient ($\log P$), boiling point (BP), enthalpy of formation (ΔH_f), and entropy (S) using theses two graph energies. We also found correlation coefficients of the physicochemical properties and molecular descriptors of BHa corresponding to the two graph energies $E(\Gamma)$ and $E_w(\Gamma)$.

Author contributions

All authors contributed equally to this paper. All authors have read and approved the final version of the manuscript for publication.

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

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Conflict of interest

The authors declare that they have no known competing financial interests.

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Appendix

```
Input: Python code to calculate eigenvalues and energy of graph

import numpy as np\\
from numpy.linalg import eig\\
def calculate energy(matrix):\\
    Convert the input to a numpy array\\
    a = np.array(matrix)\\
    Calculate eigenvalues and eigenvectors\\
    w, v = eig(a)\\
    Calculate the energy as the sum of the absolute values of
    the eigenvalues energy = np.sum(np.abs(w))\\
    return w, energy\\
Define the matrix\\
matrix = [[2, -2, 0, 0],
          [-2, 8, -3, -3],
          [0, -3, 5, -2],
          [0, -3, -2, 5]]}

Call the function and print the results\\
eigenvalues, energy = calculate energy(matrix)\\
print("Eigenvalues of the matrix:", eigenvalues)\\
print("Energy of the matrix:", energy)
```